

ME 430/529 – Advanced Energy Systems

Autumn, 2017

Overview

Energy is one of the key drivers for the modern economy. Our energy industry is based on processes that take raw energy resources found in nature (fuels, wind, sunlight, hot geothermal masses) and transform these into forms useful to the economy (electricity, mechanical power, space and process heating). Much of the study of energy focuses on the relationship between heat and work, although it is broader than this.

Modern energy systems are very complex in design. The figure on the following page shows the general flow diagram for a General Electric Class H combined cycle system. These kinds of natural gas fired plants are a significant fraction of the energy technology systems being sold today (here, the transformation is from natural gas fuel to electricity). There are sound technical reasons why this plant is configured as it is, generally focusing on achieving a very high efficiency. This particular design converts 60% of the fuel heating value to electricity (by contrast, a coal-fired Rankine cycle generally has around a 37% efficiency). The big question from the students' perspective should be why the design looks as it does, and what methodology does one use to arrive at such a design. This is the root goal of this course.

More specifically, the objectives are:

1. Understand and apply the principles used to find, quantify, and minimize the thermodynamic irreversibilities that occur in these systems. Designing to remove or minimize these is how the engineer is able to reach high efficiency.
2. Ability to use professional grade tools to make these evaluations. This is where we will replace the very simple cycle analysis procedures you used in your undergraduate thermodynamics class (*e.g.*, air standard assumptions, virtual cycles) with more accurate performance evaluation procedures.
3. Survey the major existing and evolving technologies, partly so you will have seen them, and partly using them as case studies to illustrate the preceding two items.

The principles we use to understand cycle design are based on the First and Second Laws. It's worth repeating what they offer in words at this point.

The First Law essentially says that any imbalance in the flow of energy in or out of a system must show up as a change in the energy content of the system (*e.g.*, if more heat flows into a box than leaves it, the box gets hot). This is the same as a checking account for energy. That's fundamentally all there is to it. The rest is just very accurate record keeping.

The Second Law can be stated in a practical way via the following three observations:

- Work represents the transfer of organized energy (*e.g.*, all the molecules moving in an organized direction, as in a rotating shaft). It is more valuable to us than thermal energy, in which the energy is contained in random molecular motions. Work can be directly used to perform useful tasks because the organized motion can be converted into useful tasks such as lifting weights or running a generator.

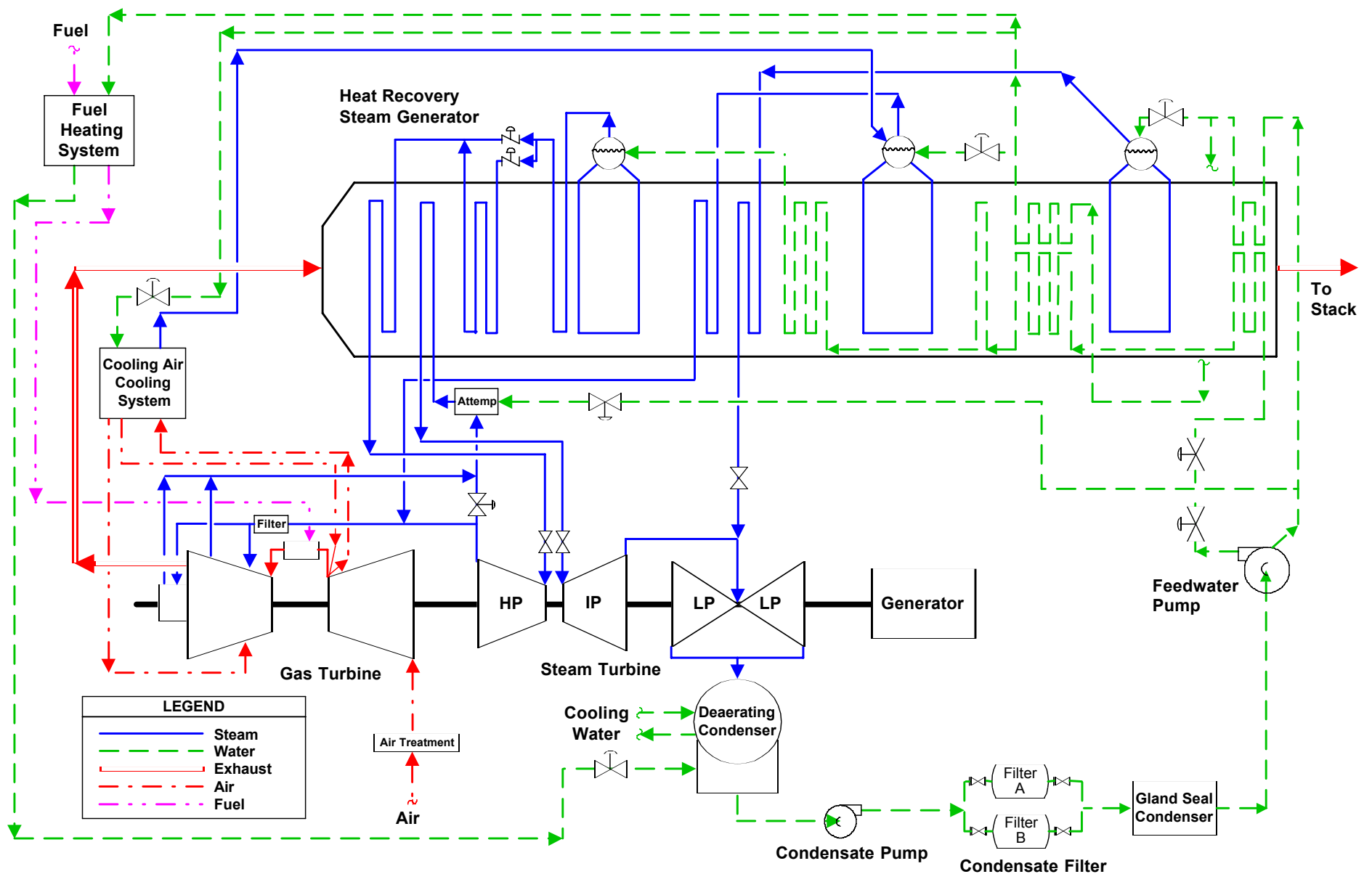


Figure 2. STAG 107H/109H cycle diagram

- A given amount of thermal energy at a higher temperature is more valuable (*i.e.*, it can be used to make more work) than the same amount of energy at a lower temperature. This is not intuitive, but it is nonetheless true.
- All real processes move in a direction that degrades the utility of the energy for making work. In other words, organized motion tends to become disorganized/randomized into thermal motion.

These imply the following:

- A portion of the work going into any real process is lost to thermal energy (*e.g.*, friction). This cannot be completely recovered as work and is lost.
- Heat always flows from hot to cold, unless helped by work to go the other way. Moving from hot to cold degrades its utility.
- Power cycles extract thermal energy from a high-temperature reservoir. Part of this is "promoted" by being converted into work (organized energy). This can only be accomplished by moving the rest of this extracted thermal energy to a lower temperature (thereby degrading its utility). In real life, the lost utility of the heat going to the lower temperature exceeds the gained utility of the heat-to-work transition. Thus, while you have some work recovered, the overall work potential of the original heat extracted is reduced.
- To move heat from cold to hot requires the intervention of work. In the best possible refrigeration cycle, the amount of value gained by the energy in moving to a hotter body is exactly offset by the loss of value of the organized work used. This exact balancing of the value of energy is what defines a reversible process.

These principles are important because they are the reasons energy systems are designed in the way they are. A principal goal of this course is learn how to look at complex energy systems as structures that are designed to extract the maximum amount of work potential from a given resource. This is how professionals do performance evaluations on practical energy systems.

Now to logistics.

Lectures

Lecture notes will be posted on the class website as scanned PDF files shortly after the lecture is given. These are intended as a supplement to the lecture, not as a reason to forego the lectures.

Problem Sets

I firmly believe you only really learn and understand this material if you apply it yourself. No matter how clear the lectures or reading may seem, you don't really understand the material until you try to do something with it **on your own**. The problem sets are your principal tool to do this. While working in groups is great for achieving group-oriented goals, you miss out on the opportunity to think the problem through on your own. Although you end up with a good grade on your homework, the problem appears when you sit down to take an exam. So my suggestion is to try the problem sets on you own as much as possible.

Problem sets will be assigned periodically on the website, with due dates depending on the length of the assignment. You will be submitting these electronically via the Canvas site for the course:

<https://canvas.uw.edu/courses/1118996/>

This should also be available via MyUW.

The assignments will always be due at 4:30 PM on the due date. I will be posting solutions on the web immediately after this, so there is **no point in asking if you can turn your assignment in late**. Just chalk it up to experience. Note that many of the assignments have project-like features and generally cannot be done if you wait until the day before the due date to get started.

I do ask that you follow a few format standards when you prepare your homework. The main goal is to ensure that we can follow how you worked through the problem. Obviously, this helps us deal with grading a large class. More importantly, the work you prepare for your technical supervisors in the outside world must be clear enough so that they can follow your thinking. A few tricks will help you do this and will have a first-order impact on your initial career success. These homework format standards will appear in the "Handouts" section of the website.

We are providing access to the SDSU Thermo website that can be used for looking up properties (thus avoiding interpolations!). The link is on the "Handouts" page, and this requires you to set up an account, but it should be free. Note that this will work only from UW IP addresses.

Exams

About one week ahead of each exam, a set of learning objectives for that exam will be posted on the web. This will give information about the material to be covered, what I will be looking for on the exam, and other logistical information.

Exams, including the final, will be given on the dates indicated. **If you are committed to travel due to your work or otherwise you need to let me know as early as possible.** This will allow us to come up with a workaround.

Grading

Grading for the undergraduate (ME 430) and graduate (ME 529) sections is done separately. For such joint classes, the graduate section includes additional content, which in this case is a special project.

The grading scheme is as follows:

Undergraduate (430)

• Homework	150
• Midterms (2@100)	200
• Final	<u>150</u>
Total	500

Graduate (529)

• Homework	150
• Midterms (2@100)	200
• Final	150
• Project	<u>100</u>
Total	600

The final grades will be based on your class ranking as determined by your percentage of the 500 or 600 total points. There is neither a fixed formula relating the percentage you achieve to your grade nor a grading curve. Instead, the mean grade for each class will be based on my subjective assessment of how well the class, overall, is getting the material. The spread will be based on another subjective judgement on how your individual performance relates to the class average. The class grades will, however, be positively correlated with class rank, *i.e.*, nobody with fewer points than another person will get a better final grade. It is theoretically possible that everybody could get a 4.0.

ME 430/529 Advanced Energy Systems

Autumn 2017

Text: Any standard thermo text (*e.g.*, Cengel and Boles). Will supplement with handouts, web materials, *etc.*

Schedule: Monday, Tuesday, Wednesday, Friday
2:30 to 3:20 PM.
MTWF: MEB 248

Calendar: This indicates tentative topic coverage

Final Exam: Tuesday, December 12, 2:30 to 4:20 PM

Instructor:
Prof. John Kramlich
MEB 319
Office Hours: Monday, Wednesday 3:30-4:30 PM, Friday 9:00-10:00 AM
kramlich@uw.edu
206-543-5538

TA:
Anamol Pundle
MEB 107
Office Hours: Tuesday, 9:00-10:00 AM, Thursday, 4:00-5:00 PM
apundle@uw.edu

Website:
<http://courses.washington.edu/mengr430/au17>

	Monday	Tuesday	Wednesday	Friday
Sept.			27 Course Intro Fundamental Principles	29 Review: Rankine and Brayton Cycles
October	2 Availability, Reversible Work	3 Irreversibility & Fuels/Combustor Chemistry	4 Reacting First Law/ Equilibrium	6 Equilibrium/ Chemical Availability
	9 Combined Cycle, Basic Design	10 Combined Cycle, Brayton Portion	11 Combined Cycle, Rankine Portion	13 Combined Cycle, HRSG Design
	16 Advanced Cycles: 2 & 3 Pressure Systems	17 Combined Cycle Economics, Technology	18 US Energy Overview	20 Solid Fuel Combustion Technology/ Biomass
	23 Environmental: NOx	24 Exam #1	25 Environmental: NOx	27 Environmental: SOx
	30 Environmental: Particulate Matter	31 Environmental: Greenhouse & Sequestration	1 Nuclear: Energy Balances	3 Nuclear: Reactions
November	6 Nuclear Decay, Fission	7 Neutron Speeds/Cross Sections/ Moderation	8 Reactor Population Balances	10 Veterans Day
	13 Nuclear Reactor Design	14 Nuclear Accidents, Weapons, Proliferation	15 Raw Biomass Fuel Characteristics	17 Black Liquor Processing
	20 Combustion Fluidized Beds	21 Exam #2	22 Biomass Fuel Refining: Overview	24 Thanksgiving
	27 Fuel Cell Overview, Electrochemistry	28 Nernst Potential Overpotentials	29 PEM Stack Design	1 PEM Design & Operation
Dec.	4 Fuel Cell Types	5 Solid Oxide Cells, Integrated Systems	6 Fuel Sources: Reformers	8 Course Review

Sept 26

Welcome to Class:

Logistics:

Sent email to class list last night. Reply if

- 1) You didn't get anything, or
- 2) You want your mail notices to go elsewhere.

Website: <http://courses.washington.edu/mengr430/au07>

- Calendar
- Handouts (no texts, 2 of those) $\Rightarrow$ Need thermo book for tables -
- HW (1st due Monday)
- Notes (after lecture).

HW due 4:30 pm on due date

- $\rightarrow$ Office
- $\rightarrow$ Front Desk
- $\rightarrow$ Electronically (one small file please!)

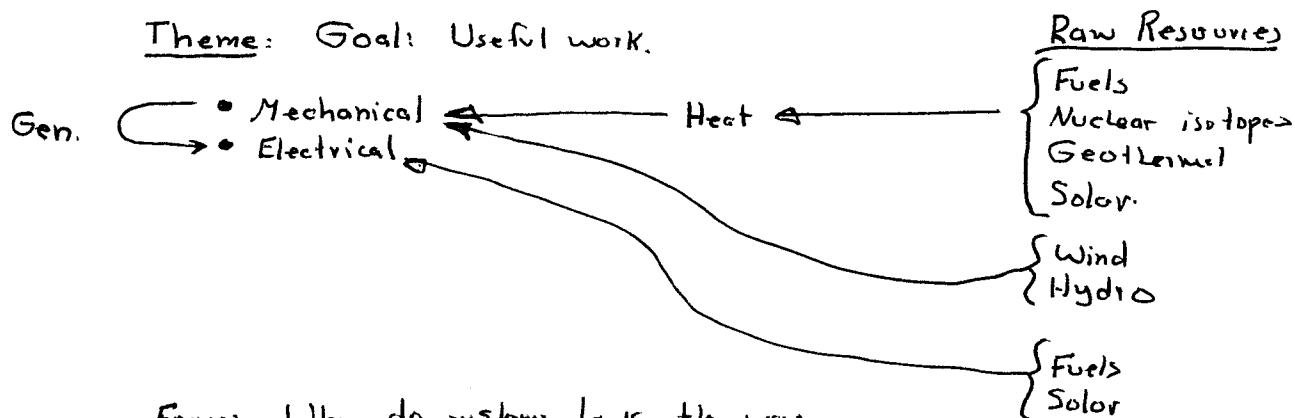
 ~~$\rightarrow$ See standards~~ $\rightarrow$ HW is Key to your understanding - ~~not~~ Ask early. $\rightarrow$ See standards.

$$Re = \frac{DV}{\gamma} = \frac{0.1m | 1m | 5}{5 | 1.E-6 m^2} = 1.0E+5$$

no surprises?

 $\rightarrow$ Keep it linear $\rightarrow$ Keep it neat!

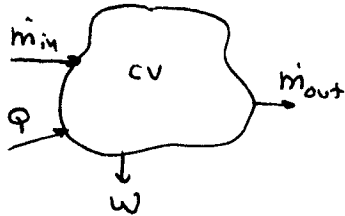
Grading - 2 mid @ 100
 HW 150
 Final 150
 500

Theme: Goals: Useful work.Focus: Why do systems look the way they do?

Topics: • Availability or Energy $\Rightarrow$ Each resource has a well-defined work potential.
 $\Rightarrow$ Recovery vs. losses

- Combined cycle systems (now)
- Next?
 - Integrated gasification combined cycle
 - Supercritical Rankine
- Nuclear
- Fuel Cells [types, H_2 -source, integration into advanced cycles].

Brief review of Energy.



Conserved Property:

Energy in - Energy out = change in CV energy
 $\Rightarrow$ like checking account.

$$\begin{array}{c} \dot{Q}, \dot{W}, \text{ flow} = u + Pv \equiv h \\ \uparrow \quad \uparrow \\ \dot{m}_{in} \quad \dot{m}_{out} \end{array}$$

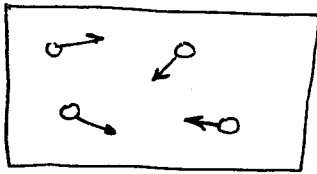
All our applications are steady state $\Rightarrow \Delta E_{CV} = 0$

$$\Rightarrow \boxed{\dot{Q} - \dot{W} = \dot{h}_{out} - \dot{h}_{in}}$$

Distinction between $\dot{Q}$ and $\dot{W}$

organized
vs.
disorganized energy.

To make it simple, think about frictionless pool table. (ideal monatomic gas)

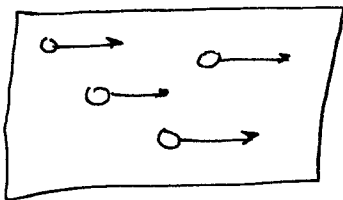


1) Only energy is in KE of balls

$$2) E = \sum \frac{1}{2}mv^2$$

3) "Gas" appears stationary but still has energy $E = u = \text{internal energy}$.

Now take same E , but make all balls go in same direction @ same speed



- Now have moving object
- Run into spring, can compress it
 $\Rightarrow$ Disorganized situation cannot.

$\Rightarrow$ Organized characterized by bulk motion.

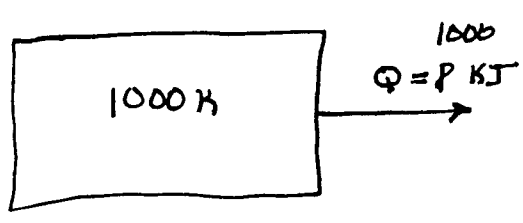
$\Rightarrow$ Thermal by molecular motion.

more useful

moved by $\dot{W}$
moved by $\dot{Q}$

2nd law says organized $\Rightarrow$ disorganized

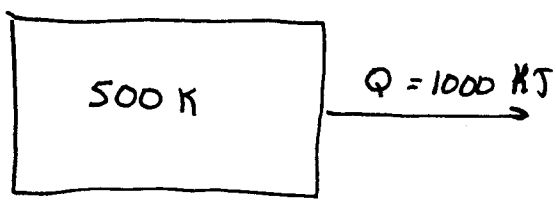
Now it turns out



Bringing two things out

- Energy of 1000 KJ
- The disorganization associated with this

$\Rightarrow \frac{1000 \text{ KJ}}{1000 \text{ K}} = 1 \text{ KJ/K} = S.$

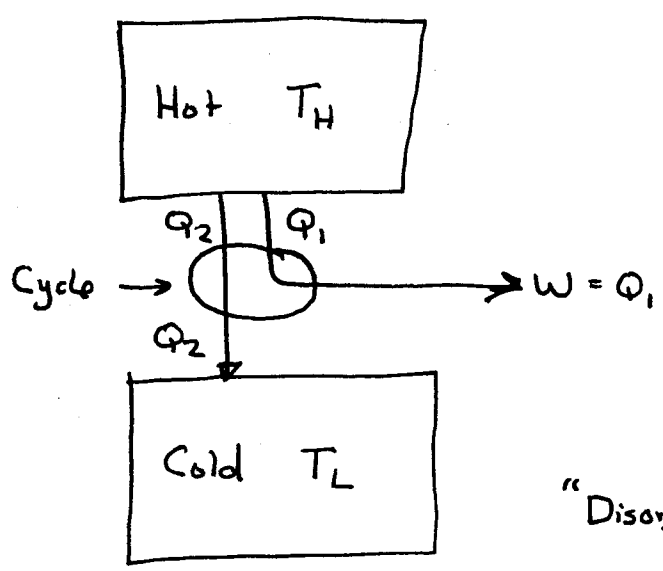


Same energy

- More disorganization

$\frac{1000 \text{ KJ}}{500 \text{ K}} = 2 \text{ KJ/K} = S.$

$\Rightarrow$ Same heat moved @ higher T is more organized and useful.



W -path $\rightarrow$ Thermal energy @ $T_H \rightarrow$ organized energy Promotion

Q_2 -path $\rightarrow$ Thermal energy @ $T_H \rightarrow$ Thermal energy @ T_L Demotion

$\Rightarrow$ Best you can do is have both "promotion" = "demotion"

$\Rightarrow$ Reversible

"Disorganization" lost by H

$$\frac{Q_1 + Q_2}{T_H} = \frac{Q_2}{T_H}$$

"Disorganization" gained by L

Equal:

$$\frac{Q_1 + Q_2}{T_H} = \frac{Q_2}{T_L}$$

$$\frac{T_L}{T_H} = \frac{Q_{in} - W}{Q_{in}} \Rightarrow \frac{W}{Q_{in}} = 1 - \frac{T_L}{T_H}$$

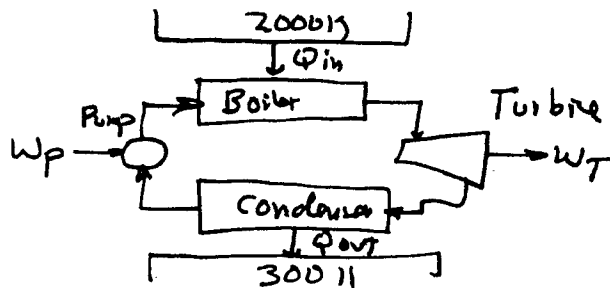
Carnot η

What we

Key points: • Hot sources provide $\dot{Q}$ with more organization
• We work to design systems that preserve this.

Now we will trash the utility of the Carnot Cycle (but it's not wrong!)

Traditional Analysis: Rankine

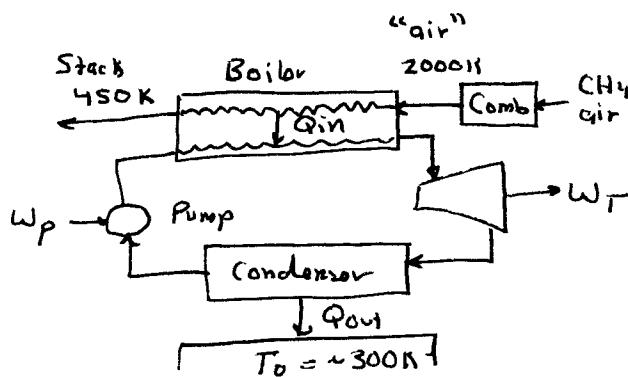


Calculate $\frac{W_{net}}{Q_{in}} = \eta_{cycle}$

Compare to Carnot

$$\frac{W_{max}}{Q_{in}} = 1 - \frac{T_L}{T_H}$$

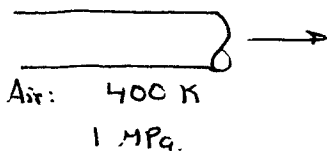
But real life looks like:



- Gas cools as it supplies heat
- No constant - T High - T reservoir
- Carnot not a realistic upper limit. (too high).

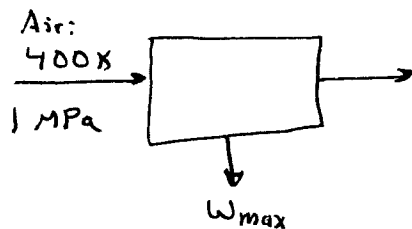
Sept. 27

Replace Carnot with Availability as an upper limit.



Air: 400 K
1 MPa.

- This is a resource for making work.
- It's utility arises because it is out of thermal and mechanical equilibrium with the environment.
- What is the upper limit on W (kJ/kg air)?



Will get W_{max} when

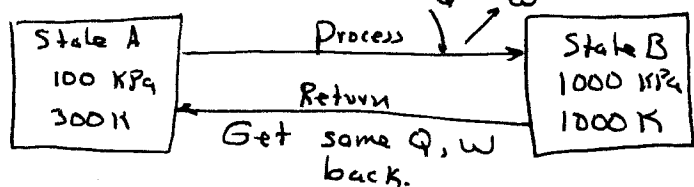
- 1) Take air to 300 K, 100 kPa.
- 2) Do this reversibly.

This makes sense because

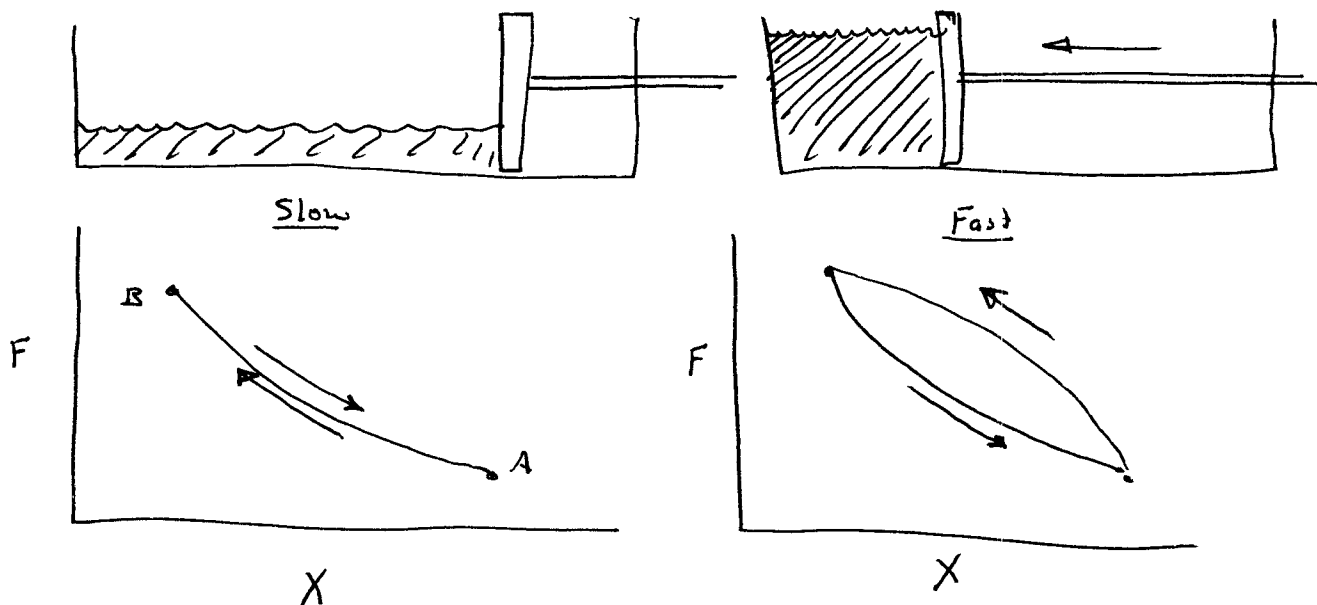
- 1) If you stop short, could get more
- 2) ~~Max work~~ Reversible processes always give you max work.

(5)

Short detour on Reversible Processes.



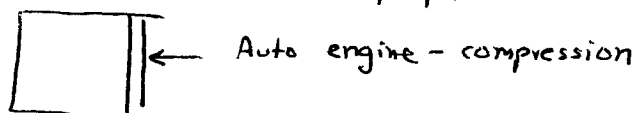
Both system and surroundings returned to same state
 (no new disorder).



- More work in
- Less work out
- Where did ΔW go? $\Rightarrow$ Thermal energy in water
- Must extract Q to return to state.
 $\Rightarrow$ net result is $W \rightarrow Q$.

Main sources of irreversibility.

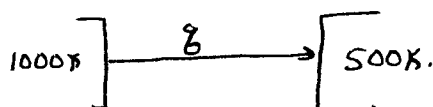
- 1) Non quasi-steady process (doing things so fast that system can't keep up).



- What do you think would be a speed where this starts to become important? $M > 0.3$
- Max piston speed @ 6000 rpm $\Rightarrow M \approx 0.15$
 $\Rightarrow$ Least common i in our world

- 2) Friction

- 3) Heat across a ΔT



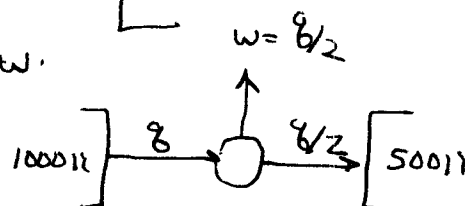
- Clearly won't return without W .

- Could intercept with carnot

$\Rightarrow$ Major

$\Rightarrow$ Design to minimize ΔT

$\Rightarrow$ Insert cycles to intercept Q .



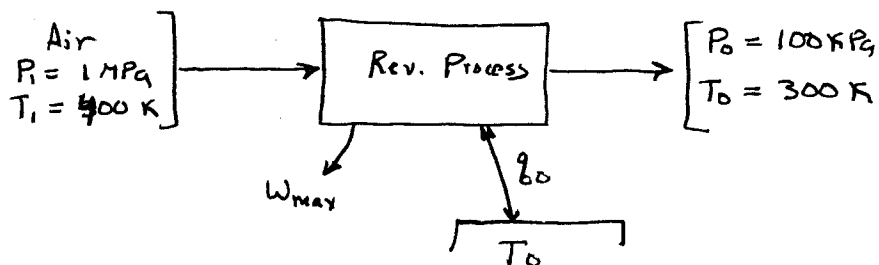
4) Unrestrained chemical reaction.

Returning to our Rankine cycle, want to replace Carnot with.

$$\eta = \frac{w_{\text{Rankine}}}{w_{\text{max for 2000 K air}}}$$

Later $\eta = \frac{w_{\text{Rankine}}}{w_{\text{max for CH}_4/\text{air @ 300K}}$

Getting w_{max} :



Best part is no need to specify process:

1st Law: $q_0 - w_{\text{max}} = h_0 - h_1 \Rightarrow w_{\text{max}} = h_1 - h_0 + q_0$

Entropy balance:

$$S_1 - S_0 + \frac{q_0}{T_0} + \cancel{S_{\text{rev}}} = \cancel{\Delta S_{\text{cv}}} \quad \begin{array}{l} \text{Reversible} \\ \text{steady state} \end{array}$$

$$\Rightarrow q_0 = -T_0 (S_1 - S_0)$$

so:

$$w_{\text{max}} = h_1 - h_0 - T_0 (S_1 - S_0)$$

Availability of our air to do work

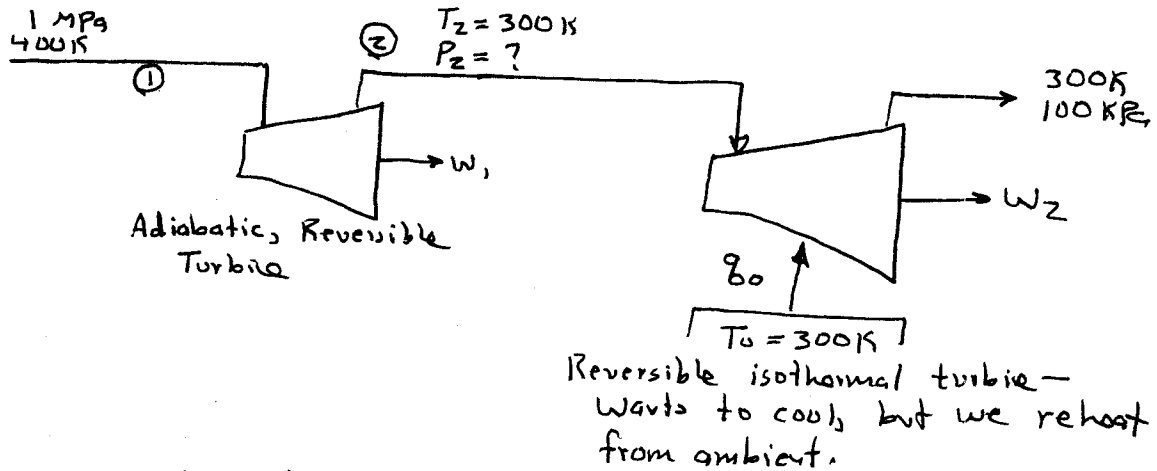
Let's run the calculation for review [constant C_p assumption].

$$\begin{aligned} w_{\text{max}} &= C_p (T_1 - T_0) - T_0 \left[C_p \ln \frac{T_1}{T_0} - R \ln \frac{P_1}{P_0} \right] \\ &= (1.005 \frac{\text{kJ}}{\text{kg} \cdot \text{K}}) (400 - 300 \text{ K}) - (300 \text{ K}) \left[(1.005 \frac{\text{kJ}}{\text{kg} \cdot \text{K}}) \ln \frac{400}{300} - (0.287 \frac{\text{kJ}}{\text{kg} \cdot \text{K}}) \ln \left(\frac{1000}{100} \right) \right] \end{aligned}$$

$$w_{\text{max}} = 212. \text{ kJ/kg}$$

Equation holds for all systems, including reacting.

Don't need to specify a process, but let's think of one



$$W_1 = C_p(T_1 - T_0)$$

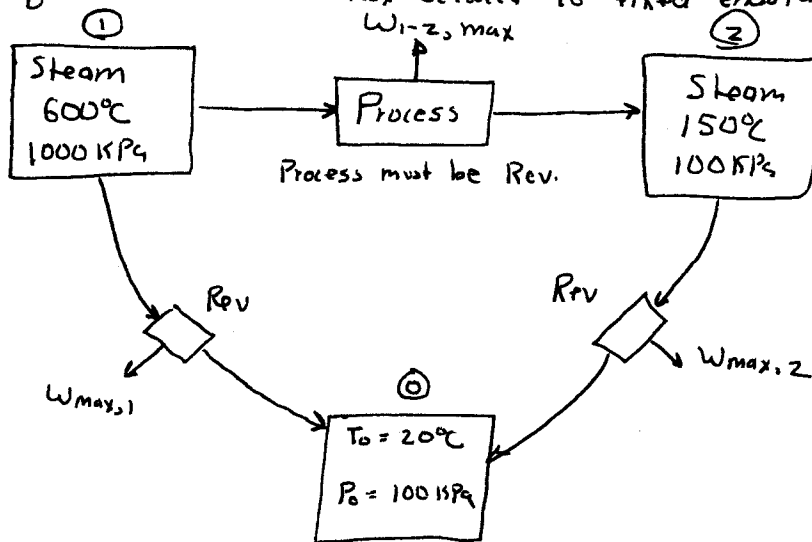
2nd Turbine: 1st Law $q - w = h_0 - h_2 = C_p(T_0 - T_2)$ for ideal gas

Entropy balance: $S_2 - S_0 + \frac{q_0}{T_0} + \cancel{\sigma_{cv}} = 0 \Rightarrow q = w$ no help

$$q = T_0(S_0 - S_2) = T_0 \left[C_p \ln \frac{T_0}{T_2} - R \ln \frac{P_0}{P_2} \right] = W_2$$

$$W = W_1 + W_2 = 212 \frac{\text{KJ}}{\text{kg}}$$

Next question: What is $W_{\max}$ between two fixed end states?



But $W_{\max,1} = W_{\max,1-2} + W_{\max,2}$

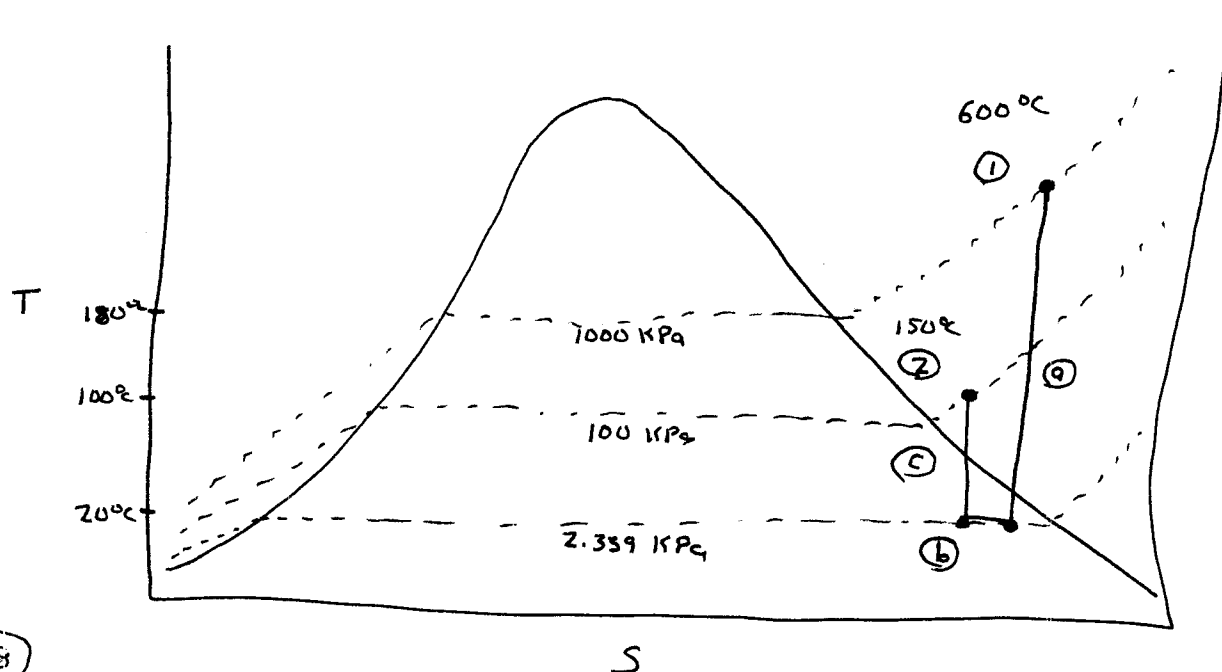
$\Rightarrow W_{\max,1-2} = W_{\max,1} - W_{\max,2}$ which we know.

$$W_{1-2} = [h_1 - h_0 - T_0(S_1 - S_0)] - [h_2 - h_0 - T_0(S_2 - S_0)]$$

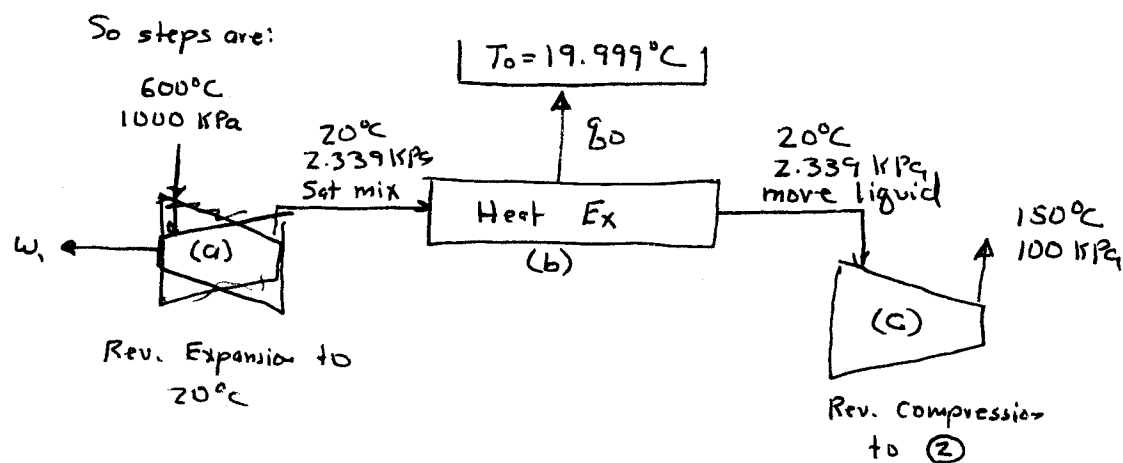
$$W_{\text{rev}} = h_1 - h_2 - T_0(S_1 - S_2)$$

Values from steam table give
= 799.7 KJ/kg steam

Question: Why does this depend on T_0 ? Seems like answer should be same on Earth as Mars.



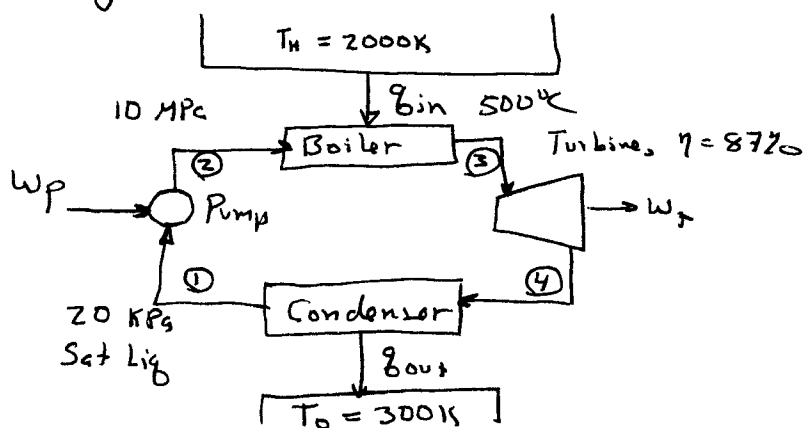
Sept. 28



T_0 impacts each process

Last item is irreversibility.

Develop via example:
Traditional Rankine



• Given this you can do the standard cycle calculations $\rightarrow W_{net} \text{ (kJ/kg)}$

• Best cycle is Carnot

$$w_{max} = q_{in} \left[1 - \frac{T_0}{T_H} \right]$$

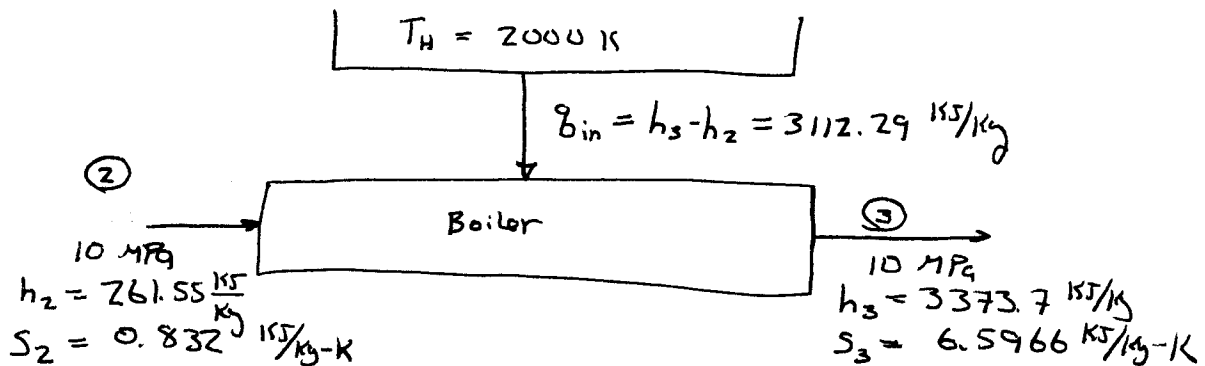
• $i = w_{max} - w_{act}$ Possible work that is lost due to cycle irreversibilities

$\Rightarrow$ But where do these occur?

How many?

- 1) Boiler (q across ΔT)
 - 2) Turbine (friction)
 - 3) Condenser (q across ΔT)
- $$\left. \begin{array}{l} 1) \text{ Boiler } (q \text{ across } \Delta T) \\ 2) \text{ Turbine (friction)} \\ 3) \text{ Condenser } (q \text{ across } \Delta T) \end{array} \right\} \Sigma = i$$

Derive based on boiler:



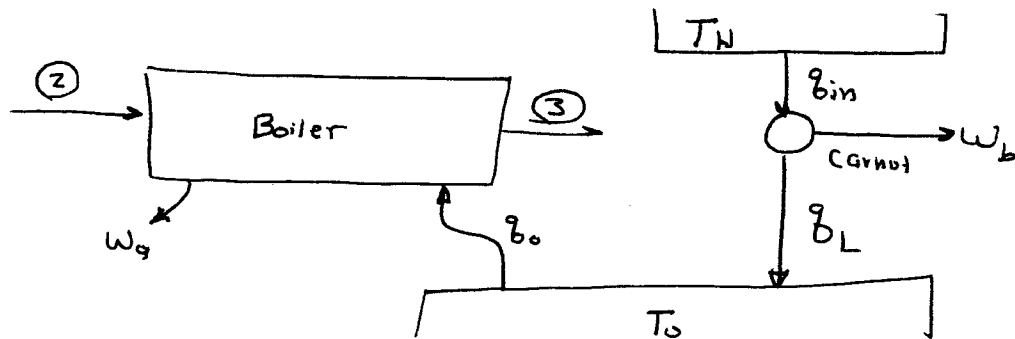
The idea is to construct a totally reversible process that does everything the real process does:

a) Reversibly convert 1 kg of steam from ② $\rightarrow$ ③

b) Reversibly remove 3112.29 kJ of heat from high-T reservoir.

$$\Rightarrow w_{max}$$

$$i = w_{max} - w_{act} \rightarrow 0 \text{ here.}$$



$$w_g \text{ we just did: } w_g = h_2 - h_3 - T_0 (s_2 - s_3)$$

$$w_b \text{ is Carnot: } w_b = q_{in} \left[1 - \frac{T_0}{T_H} \right] = q_{in} - q_{in} \frac{T_0}{T_H}$$

$$w_{max} = \underbrace{h_2 - h_3 - T_0 (s_2 - s_3)}_{\text{cancel}} + \underbrace{q_{in} - q_{in} \frac{T_0}{T_H}}_{\text{cancel}}$$

1st Law on original system is:
so these can cancel.

$$q_{in} = h_3 - h_2 \text{ or } q_{in} + (h_2 - h_3) = 0$$

Customary to reference q to reservoir:

$$q_{in} = -q_R$$

$$\Rightarrow W_{max} = T_0 \left[S_3 - S_2 + \frac{q_R}{T_R} \right]$$

$$\dot{i} = W_{max} - W_{act}$$

$$\Rightarrow \boxed{\dot{i} = T_0 \left[S_{exit} - S_{inlet} + \frac{q_R}{T_R} \right]}$$

Sign on q is referenced to reservoir

- + if into res
- if out.

In handout we work through cycle $\Rightarrow h, s$ at each point.

$$q_{in} = 3112 \text{ kJ/kg}$$

$$q_{out} = 2077 \text{ kJ/kg}$$

$$W_{net} = 1035 \text{ kJ/kg}$$

$$\dot{i}_{1-2} = 0$$

$$\dot{i}_{2-3} = T_0 \left(S_3 - S_2 + \frac{q_R}{T_R} \right) = [300] \left[6.5966 - 8.32 + \frac{-3112}{2000} \right] = 1263 \text{ kJ/kg}$$

$$\dot{i}_{3-4} = T_0 (S_4 - S_3) = 141$$

$$\dot{i}_{4-1} = T_0 \left[S_1 - S_4 + \frac{q_{out}}{T_0} \right] = 207$$

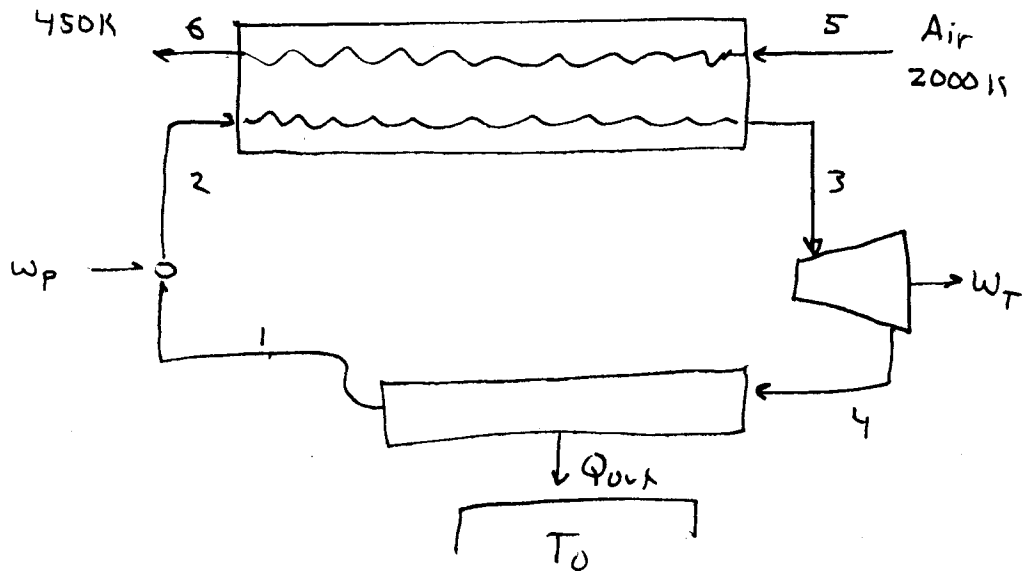
$$\text{Carnot says: } W_{max} = q_{in} \left[1 - \frac{T_0}{T_h} \right] = 2645$$

Payoff:

W_{net}	1035	39.1
i : boiler	1263	47.7
turbine	141	5.3
condenser	207	7.9
	<u>2646</u>	

Accounted for all work potential.

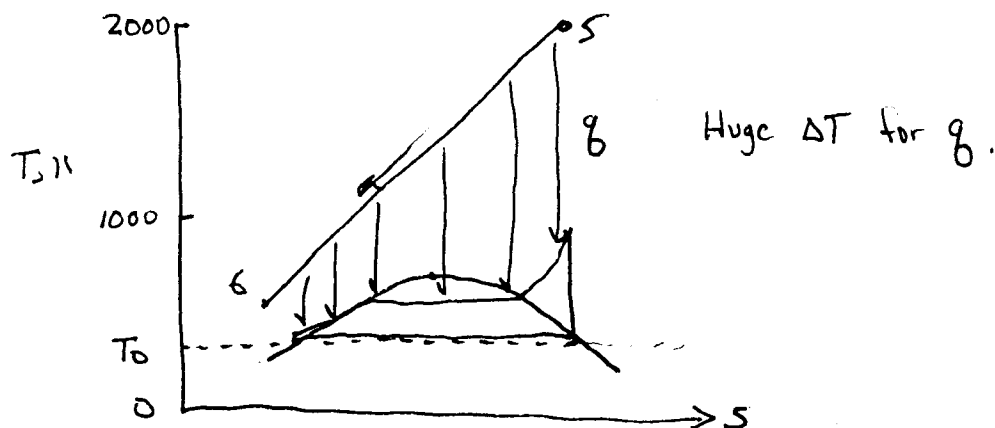
Now compare to real cycle:



Differences:

- 1) W_{max} = availability of air @ ⑤
 - 2) $i_{boiler} = T_0 [\dot{m}_a (S_5 - S_6) + \dot{m}_{s2} (S_3 - S_2)]$ Note: No g term since it's internal.
 - 3) Work lost with 6 $\Rightarrow$ Avail of air @ ⑥
- so: $W_{max,5} = W_{net} + W_{lost,6} + \sum i's$ (3)

Boiler is still bad actor:

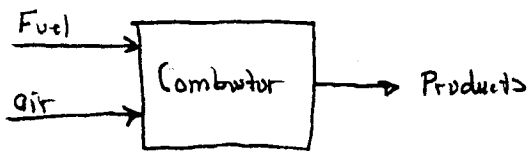


Summary:

- Three concepts:
 - Availability
 - W_{max} ① $\rightarrow$ ②
 - i = lost work.
- What is reversibility?
- What are four types of i ?

Chemistry $\rightarrow$ i, w_{max} for reacting systems.

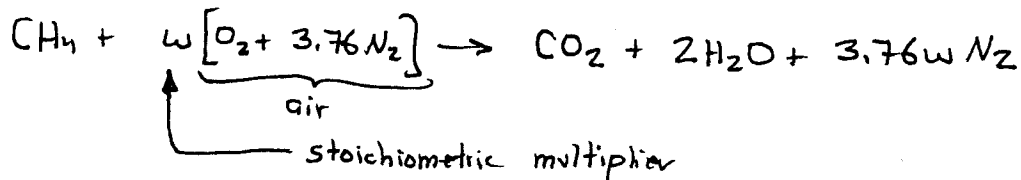
Three topics:
 • Stoichiometry
 • 1st Law for reacting $\left. \begin{array}{l} \text{Stoichiometry} \\ \text{1st Law for reacting} \end{array} \right\} \text{Review}$
 • Equilibrium $\rightarrow$ Chem availability, w_{max} for gallon of gas.



Stoichiometric Combustion:

Just enough air for:
 $C \rightarrow CO_2$
 $H \rightarrow H_2O$
and no left-over O_2 .

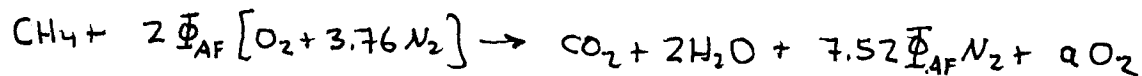
CH_4 : Choose 1 kmole as basis and stick with it:



Get w by balancing O-atoms: $2w = 2 + 2 \Rightarrow \boxed{w = 2}$

$\Rightarrow$ Stoichiometric is $CH_4 + 2[O_2 + 3.76 N_2] \rightarrow CO_2 + 2H_2O + 7.52 N_2$

Now allow for excess air [the usual case]



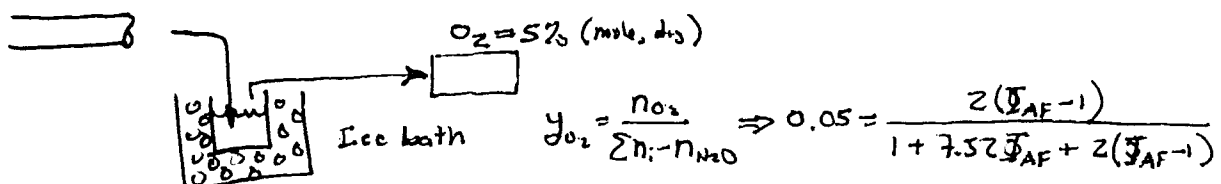
$\Phi_{AF} \equiv$ air/fuel equivalence ratio $\Rightarrow \begin{cases} = 1 @ \text{stoichiometric} \\ > 1 \text{ for fuel-lean} \end{cases}$

Get "a" from O-atom balance: $4\Phi_{AF} = 2 + 2 + 2a \Rightarrow a = 2[\Phi_{AF} - 1]$

always $a = w[\Phi_{AF} - 1]$

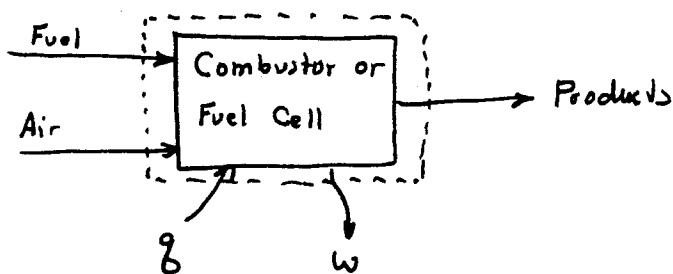
Two most common calculations are:
 1) Know fuel & air flows $\rightarrow$ Get Φ_{AF} , $\rightarrow$ Get product gas comp.
 2) Measure product gas comp $\rightarrow$ Get Φ_{AF}

ME Engine exhaust:



$\Rightarrow \Phi_{AF} = 1.2795 \Rightarrow 127.95\% \text{ Theoretical air}$
 $\Rightarrow 27.95\% \text{ Excess air}$

Now to 1st Law:

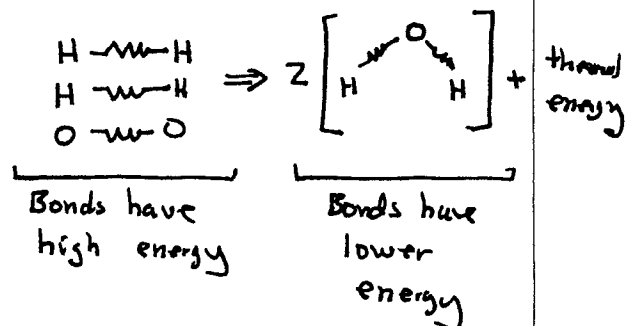
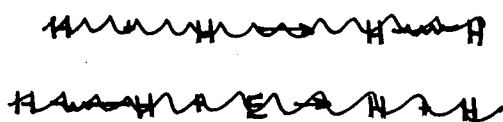


$$q - w = H_P - H_R$$

- On h's. We generally are interested in Δh , so tables are built using an arbitrary zero point.

$$h \equiv 0 \begin{cases} \text{Air: } 0 \text{ K} \\ \text{Steam: liquid water @ } 0^\circ\text{C} \end{cases}$$

- For reacting systems, need to include
 - Thermal energy
 - Potential energy in bonds.



- Cover this by $h \equiv 0$ for - elements in standard state (O_2, H_2) - 25°C

- So for CO_2 @ 700 K:

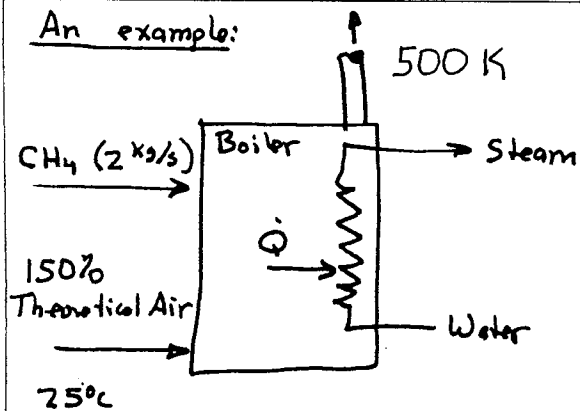
$$h_{\text{CO}_2} = \underbrace{h_{f,\text{CO}_2}^\circ}_{\substack{\Delta h \text{ for } \text{C} + \text{O}_2 \\ \rightarrow \text{CO}_2 \text{ @ } 25^\circ\text{C}}} + \underbrace{[h - h_{298}]_{\text{CO}_2}}_{\substack{\Delta h \text{ for } \text{CO}_2 \\ 25^\circ\text{C} \rightarrow 700\text{K.}}}$$

or

$$-379,759 \frac{\text{kJ}}{\text{kmole CO}_2} = -393,520 + 27,125 - 9364 \frac{\text{kJ}}{\text{kmole CO}_2}$$

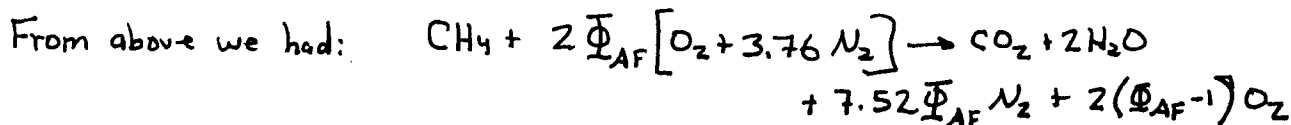
since $h \neq h(P)$ for an ideal gas, this is it for finding h of any compound @ any T .

$\Rightarrow$ 1st Law is: $q - w = \sum_P n_i h_i - \sum_R n_i h_i$

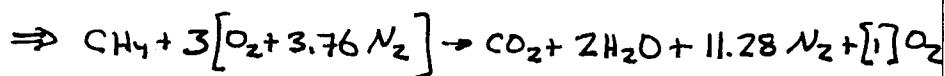


$$\dot{Q} = ?$$

Hint: Choose 1 kmole CH₄ as a basis and adjust @ end of problem to real CH₄ flow.



Here, $\Phi_{AF} = 1.5$



	Species	Kmoles	h_f°	$h - h_{298}$	$n_i [h_f^\circ + h - h_{298}]$	
R	CH ₄	1	-74,850	0	-74,850	$\Sigma = H_R$ = -74,850
	O ₂	3	0	0	0	
	N ₂	11.28	0	0	0	
P	CO ₂	1	-393,520	17,678 - 9364	-385,206	$\Sigma = H_P$ = -782,223
	H ₂ O	2	-241,820	16,828 - 9904	-469,792	
	N ₂	11.28	0	14,581 - 8669	+66,687	
	O ₂	1	0	14,770 - 8682	+6,088	

$$\dot{Q} = H_R - H_P = [-782,223] - [-74,850] = -707,373 \frac{\text{KJ}}{\text{kmole CH}_4}$$

Finally correct to real flow:

$$\frac{-707,373 \text{ KJ}}{\text{kmole CH}_4} \times \frac{\text{kmole}}{16 \text{ kg}} \times \frac{2 \text{ kg}}{\text{s}} = \boxed{-88,422 \text{ KW}}$$

If $\dot{Q} = 0$, how do I get T_P ?

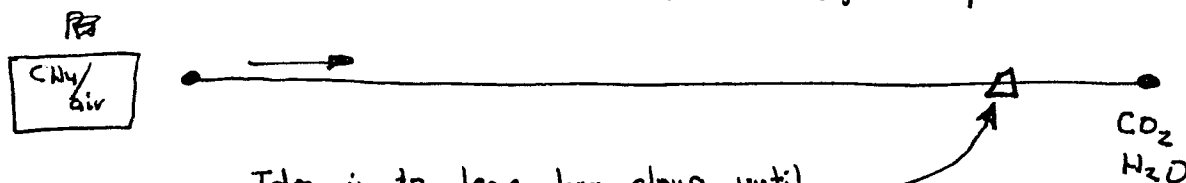
Equilibrium - Chemical Availability.

If you run the calc for T_P for $\Phi = 1$ CH₄ + air $\Rightarrow T_P = 3300 \text{ K}$.

But experiment says $T_P \approx 2200 \text{ K}$. What's going on?

- Products are partly dissociated $\text{CO}_2 \rightarrow \text{CO} + \frac{1}{2} \text{O}_2$ (endothermic, so T_P comes down).

H₂, OH, O,
H₂, NO,
etc.

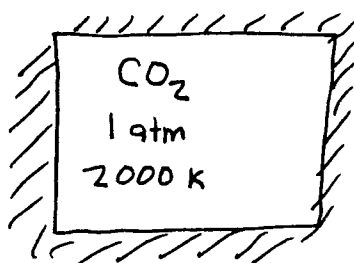


Idea is to leave box alone until spontaneous rxn stops

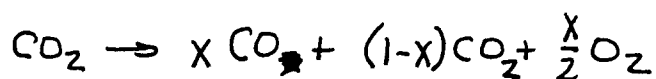
Oct. 3

Aside: Rule of thumb: $T_p < 1200\text{ K}$, no significant dissociation
 $> 1200\text{ K}$, it becomes a problem.

How to do it? Make use of the fact that we are looking for point where spontaneous reaction stops.



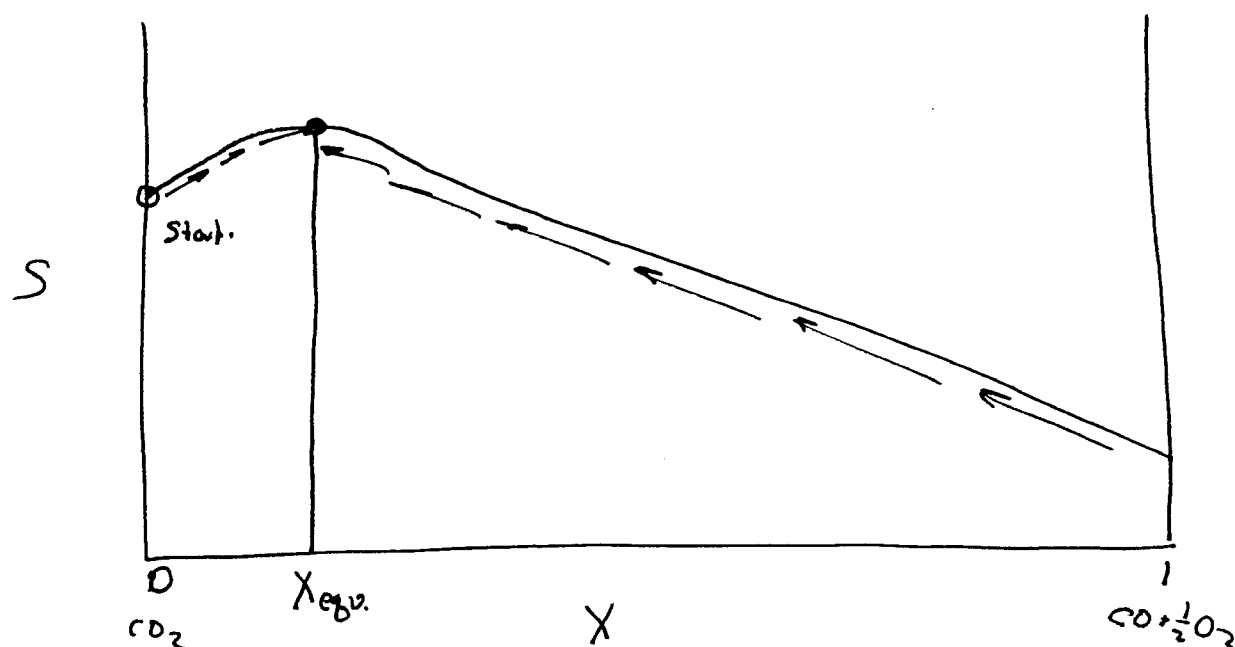
Rigid, insulated box.



$X=0 \Rightarrow \text{all CO}_2$
 $X=1 \Rightarrow \text{CO} + \frac{1}{2} \text{O}_2$

All values between are possible.

If you give me X , I can calculate $S = \sum n_i s_i = \sum n_i \left[S_i^\circ - R \ln \frac{P_i}{P_0} \right]$
 (with some work).



Why did we do this? Let's do entropy balance on CV.

In - Out + Source = accumulation

$$\sigma_{\text{CV}} = \Delta S_{\text{CV}} \quad \left| \quad \begin{array}{l} \text{2nd Law says } \sigma_{\text{CV}} > 0 \text{ for} \\ \text{spontaneous process, so} \\ \text{process will only go if} \\ \Delta S_{\text{CV}} > 0. \end{array} \right.$$

$\Rightarrow$ Reaction will proceed until S_{max} , and then get stuck.

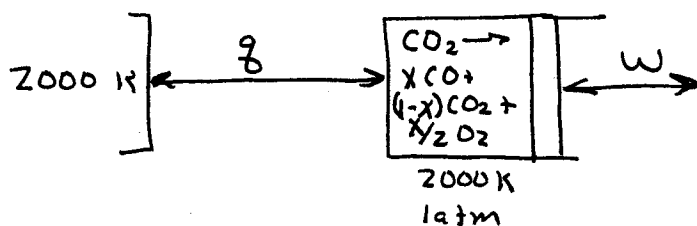
$\Rightarrow$ Could start from other side, and will get same answer

$\Rightarrow$ As we approach equilibrium, $T \downarrow$ (endothermic)

$\Rightarrow P, T$ are part of answer. $P \uparrow$ ($\text{CO}_2 \rightarrow \text{CO} + \frac{1}{2} \text{O}_2$) (probably)

More often than not, interested in known P, T (e.g. gas turbine combustor outlet is 8 atm, 1600K). $\Rightarrow$ Want comp, h, s .

Thermodynamically, this idealizes to:



as X goes from

$0 \rightarrow X_{\text{final}}$

- 1) Piston moves to keep $P = 1 \text{ atm}$
- 2) Heat flows to keep $T = 2000 \text{ K}$

Entropy balance $\frac{q}{T} + \sigma_{cv} = \Delta S_{cv}$ or $\frac{\delta q}{T} + \delta \sigma_{cv} = dS_{cv}$

Since $\sigma_{cv} \geq 0$ for spontaneous process

$$\frac{\delta q}{T} \leq dS \quad \text{or} \quad \delta q \leq T dS$$

1st Law $\delta q - \frac{\delta w}{P dV} = du \Rightarrow T dS - P dV \geq du$

or $0 \geq du + P dV - T dS$

Define Gibbs $g \equiv u + P v - T s = h - T s$

$$dg = du + P dv + v dP - T ds - s dT \quad \text{const } P, T.$$

$\Rightarrow$

$0 \geq dg$ for spontaneous process @ fixed P, T .

$\rightarrow$ Equilibrium occurs @ $dg = 0$ (like $ds = 0$ before)

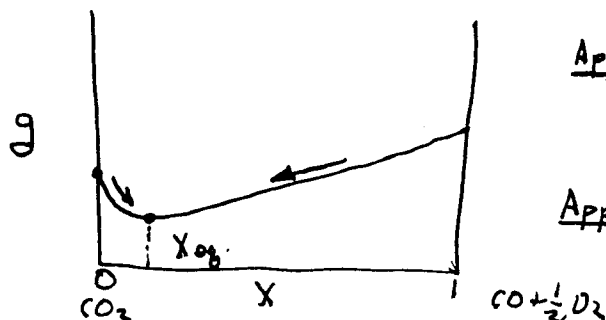
$\rightarrow$ This will be @ a minimum in g .

$$g = \sum n_i g_i \quad g_i = h_f^\circ + h_i - h_{298} - T \left[S_i^\circ - R \ln \frac{P_i}{P_0} \right]$$

all can be looked up.

$$X \rightarrow n_i \\ T, P, X \rightarrow g_i$$

How to calculate?



Approach 1: Equilibrium constants $\rightarrow$ Developed in thermo book... Good for hand calculations

Approach 2: General Gibbs minimization.
 $\rightarrow$ Need code, many species
 $\rightarrow$ See handout.

In broad outline:

(minimize g)

$$g = \sum n_i g_i = g_{\text{CO}_2} n_{\text{CO}_2} + g_{\text{CO}} n_{\text{CO}} + g_{\text{O}_2} n_{\text{O}_2}$$

$$g_{\text{CO}_2} = h - Ts = h_f^\circ + h - h_{298} - T \left[S^\circ - R \ln \frac{P_{\text{CO}_2}}{P_0} \right]$$

$$= \underbrace{h_f^\circ + h - h_{298} - TS^\circ}_{\equiv g_{\text{CO}_2}^*(T)} + RT \ln \frac{P_{\text{CO}_2}}{P_0}$$

also $\frac{P_{\text{CO}_2}}{P_0} = \frac{n_{\text{CO}_2}}{n_T} \frac{P_T}{P_0}$

so $g = \left[g_{\text{CO}_2}^* + RT \ln \left[\frac{n_{\text{CO}_2}}{n_T} \frac{P_T}{P_0} \right] \right] n_{\text{CO}_2} + \left[g_{\text{CO}}^* + RT \ln \left[\frac{n_{\text{CO}}}{n_T} \frac{P_T}{P_0} \right] \right] n_{\text{CO}} + \left[g_{\text{O}_2}^* + RT \ln \left[\frac{n_{\text{O}_2}}{n_T} \frac{P_T}{P_0} \right] \right] n_{\text{O}_2}$

Unknowns: $n_{\text{CO}_2}, n_{\text{CO}}, n_{\text{O}_2}, n_T$ but $n_T = n_{\text{CO}_2} + n_{\text{CO}} + n_{\text{O}_2}$

So have 3. But these are constrained by atom balances

C: $1 = n_{\text{CO}} + n_{\text{CO}_2}$ $n_{\text{CO}_2} = 1 - n_{\text{CO}}$ let $n_{\text{CO}} = X$
 $n_{\text{CO}_2} = 1 - X$

O: $2 = n_{\text{CO}} + 2n_{\text{CO}_2} + 2n_{\text{O}_2}$
 $\underbrace{X + 2(1-X)}_{2-X} + 2n_{\text{O}_2} = 2$ $n_{\text{O}_2} = \frac{X}{2}$

so finally, $g = g(X)$ only. Take $\frac{dg}{dX} = 0 \Rightarrow \underline{X_{\text{equilibrium}}}$

Will work with ~~natural gas~~ CH_4 + air $\Rightarrow$ 50 species, 4 elements [C, H, O, N]

Make use of method of Lagrange Multipliers plus Newton-Raphson numerical solution (p. 3 $\rightarrow$ end of writeup $\rightarrow$ optional).
Inversion of 5x5 matrix

Code resides on ~~ME~~ computers $\rightarrow$ Also can download a [Windows version Plus a Mac OS9 version]

to Old Line Entry

New Menu Driven

Windows

X, Y

X = Download

Mac OS9

Y = UW-ME



Recommend because it has some more flexible capabilities (different T_f, T_o)

Oct 4

Choose an adiabatic burner running on $\text{CH}_4 + 2\text{H}_2$
 T_P , composition, h , S ,
 + 200% theoretical air

① Specify inlet comp (two steps).

[1a] Specify comp. of fuel & air streams.

"Fuel" List

	Relative Moles		
CH_4	1	or	5
H_2	2		10

"Oxidizer" List

		or	
O_2	0.21		1
N_2	0.79		3.76

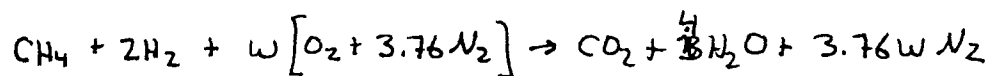
• Just sets internal composition of fuel & air streams

• We'll set fuel vs. air next.

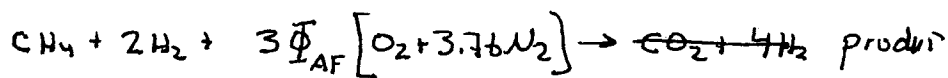
[1b] Set ratio of air/fuel $\Rightarrow$ Several Ways.

• $\Phi_{AF} = 1/\Phi_{FA} = 0.5$

• kg air/kg fuel:



$$2w = 2 + 4 \Rightarrow w = 3$$

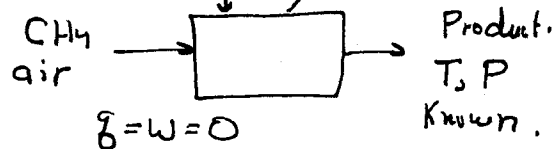


$$\underbrace{m_f = 16 + (2)(2)}_2 \quad \underbrace{m_{ox} = 3 \cdot 2 \cdot [32 + (3.76)(28)]}_1$$

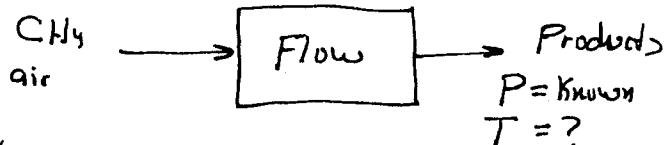
$$\frac{m_{ox}}{m_f} = 41.18$$

② Choose problem type:

3 most common:

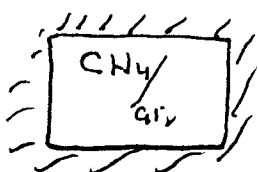


"TP"



"HP"

($H_P = H_R$)



$$q = 0$$

$$V = \text{const.}$$

$$\Rightarrow \text{Products}$$

$$P = ?$$

$$T = ?$$

"LV"

$$u = \text{const.}$$

$$V = \text{const.}$$

③ Choose parameters

$$\begin{array}{ll}
 TP \rightarrow \begin{array}{l} \text{Input} \\ \text{known} \end{array} \text{ final } T, P & \\
 HP \rightarrow \text{Inlet } T, P & T \Rightarrow h_R = h_P \text{ held constant} \\
 UV \rightarrow \text{Inlet } T, P & \left. \begin{array}{l} T \Rightarrow u_R = u_P \\ P \Rightarrow V_R = V_P \end{array} \right\} \text{ held constant.}
 \end{array}$$

④ Run code: Output: Composition $\rightarrow$ mole fractions (get column right!)
 $h = \text{kJ/kg mix}$
 $s = \text{kJ/kg mix-K}$ } uses same basis as u , so values can be used in hand calculations.

for us: $T = \cancel{1532 \text{ K}} \quad 1536 \text{ K}$
 $h = \cancel{-88.578} \text{ kJ/kg mix} \quad -88.892$
 $s = 9.1959 \text{ kJ/kg mix-K}$

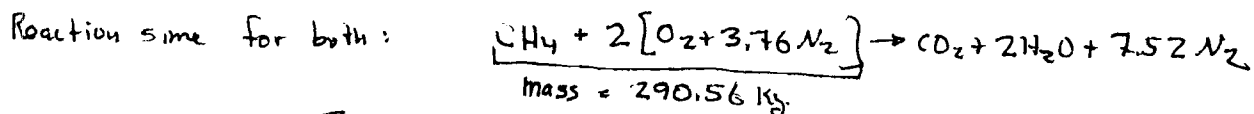
$$\frac{\text{mass mix}}{\text{kmole fuel}} = 16 + (2)(2) + 6[(32) + (3.76)(28)] = 843.68 \frac{\text{kg mix}}{\text{kmole CH}_4}$$

$$\begin{aligned}
 \Rightarrow h &= \frac{-\cancel{88.578} \text{ kJ}}{\text{kg mix}} \left| \frac{843.68 \text{ kg mix}}{\text{kmole CH}_4} \right| = \frac{-74,990}{\cancel{74,748} \text{ kJ/kmole CH}_4} \\
 &= h_{f, \text{CH}_4}^{\circ} \quad (\text{not a coincidence, why?})
 \end{aligned}$$

Now we can do chemical availability. $\Rightarrow$ See handout.

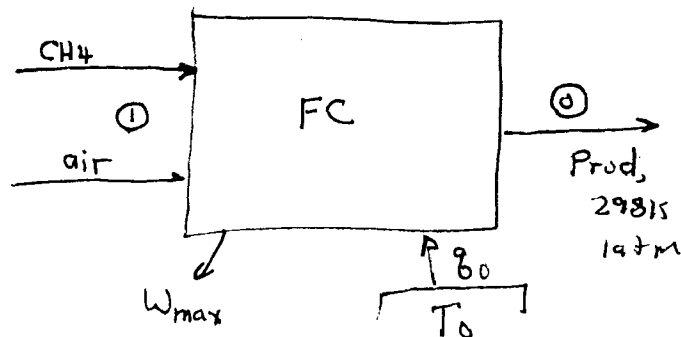
Start with 1 kmole CH_4 + stoichiometric air

- $W_{\max}$ for fuel cell.
- Burn CH_4 ; then recover heat reversibly.



$$T_0 = 298 \text{ K}$$

$$P_0 = 1 \text{ atm}$$



$$W_{\max} = h_1 - h_0 - T_0 (s_1 - s_0)$$

Gr

Get h_i the usual way:

Species	Kmol/s	h_f°	$h - h_{f,ss}$	$n_i [h_f^\circ + h - h_{f,ss}]$	S°	P_i (atm)	S_i
CH ₄	1	-74,850	0	-74,850	186.16	1	186.16
O ₂	2	0	0	0	205.04	0.21	218.02
N ₂	7.52	0	0	0	191.61	0.79	193.57

$$h_i = \Sigma = -74,850 \text{ kJ/kmol CH}_4$$

$$S_i = \Sigma n_i S_i; \quad S_i = S_i^\circ - R \ln \frac{P_i}{P_0} \quad \leftarrow \text{Partial Pressure of } i \text{ in mix}$$

Reference P for S° (always 1 atm)

$$S_{CH_4} = S_{CH_4}^\circ - R \ln \frac{P_{CH_4}}{P_0} = 186.16 - \left[8.314 \frac{\text{kJ}}{\text{kmol} \cdot \text{K}} \right] \ln \left[\frac{1}{1} \right]$$

$$S_{O_2} = S_{O_2}^\circ - R \ln \frac{P_{O_2}}{P_0} = 205.04 - \left[8.314 \right] \ln \left[\frac{0.21}{1} \right]$$

$$S_i = \frac{186.16}{205.04} + [2][218.02] + [7.52][193.57] = 2077.85 \frac{\text{kJ}}{\text{kmol CH}_4 \cdot \text{K}}$$

Oct 5

Next, want h_0 S_0 : Could repeat hand calc. for products, but let's use code:

$$\left. \begin{array}{l} \text{Fuel: CH}_4 \\ \text{Ox: Air} \end{array} \right| \Phi_{AF} = 1 \left| \begin{array}{l} \text{TP Problem} \\ T = 298 \text{ K} \\ P = 1 \text{ atm} \end{array} \right\} \begin{array}{l} h_0 = -3017.5 \text{ kJ/kg mix} \\ S_0 = 7.2214 \text{ kJ/kg mix} \cdot \text{K} \end{array}$$

Got "Apples" vs. "Oranges" $\Rightarrow$ Convert using $290.56 \frac{\text{kg mix}}{\text{kmol CH}_4}$

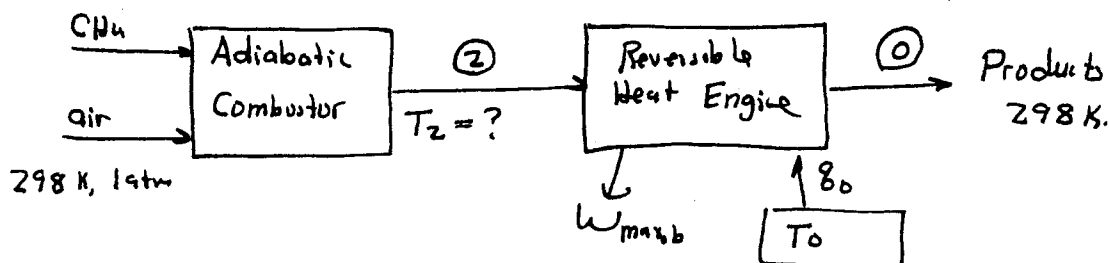
$$\Rightarrow h_0 = -876,778 \text{ kJ/kmol CH}_4$$

$$S_0 = 2098.25 \text{ kJ/kmol CH}_4 \cdot \text{K}$$

$$\Rightarrow W_{\text{max, FC}} = [-74,850] - [-876,778] - [298][2077.85 - 2098.25]$$

$$W_{\text{max, FC}} = 808,007 \frac{\text{kJ}}{\text{kmol CH}_4}$$

Now reversible combustor + heat engine.



First, let's just get state ②

$$\left. \begin{array}{l} \frac{\text{CH}_4}{\text{air}} \mid \Phi_{AF}=1 \mid \text{HP} \mid \begin{array}{l} T_R = 298 \text{ K} \\ P_2 = 1 \text{ atm} \end{array} \right\} \rightarrow \begin{array}{l} T_2 = 2226 \text{ K} \\ h_2 = -257.61 \text{ kJ/kg mix} \\ S_2 = 9.8226 \text{ kJ/kg mix} \end{array}$$

Use $290.56 \frac{\text{kg mix}}{\text{kmol CH}_4}$

Have h_0, S_0 from before $\Rightarrow W_{\max,b} = h_2 - h_0 - T_0(S_2 - S_0)$

$$\text{or } = [-74,850] - [-876,776] - [298][2854.05 - 2098.25]$$

$$W_{\max,b} = 576,700 \text{ kJ/kmol CH}_4$$

vs. $808,007 \text{ kJ/kmol CH}_4$
availability in original

Where did the missing work go?

$$\Rightarrow i_{\text{comb}} = T_0(S_2 - S_0)$$

$$= (298 \text{ K})(2854.05 - 2098.25) = 236,307 \text{ kJ/kmol CH}_4$$

and of course $236,307 + 576,700 = 808,007$!

So this is i due to unrestrained reaction.

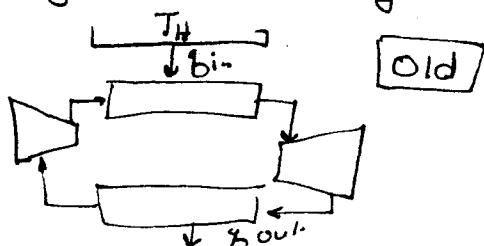
So ideal fuel cell recovers	100%
Ideal combustor + Heat engine	71.4%
	+ 28.6% irreversibility

Sometimes hear about Fuel Cells.

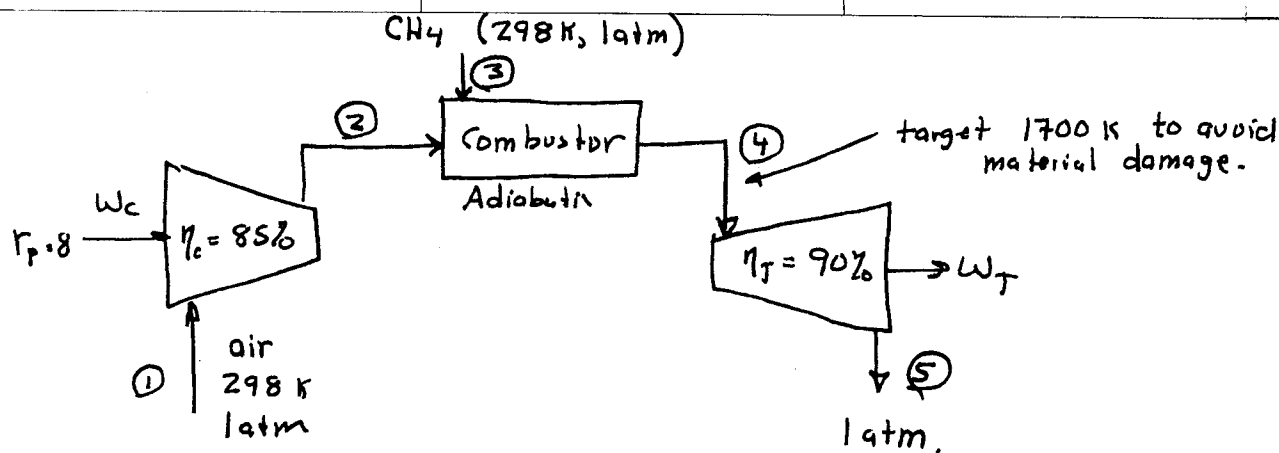
- Not bound by Carnot.
- Not a heat engine
- Not bound by 2nd Law.

} Really means they can avoid some of i_{comb} .

Now ready to do a real Brayton cycle



Core for combined cycle.



Let's analyze:

Compressor.

Same as traditional since it's just air $\Rightarrow T_2, h_2, S_2$

$$W_c = \dot{m}_a (h_2 - h_1) \text{ KJ/kg air}$$

$$\dot{Q}_c = \dot{m}_a T_0 (S_2 - S_1) \quad "$$

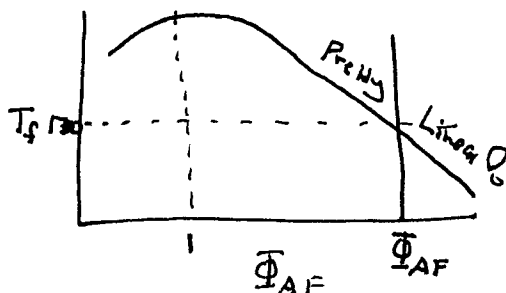
Combustor. Model outlet as equilibrium. 8 atm, 1700 K.

Now here's an issue: How do I get a targeted temperature out of an adiabatic combustor? Vary Φ_{AF}

Run HP and vary Φ_{AF} until I hit 1700 K.

$$\left. \begin{array}{l} \text{CH}_4 / \text{air} \mid \Phi_{AF} = \text{guess} \mid \text{HP} \mid \begin{array}{l} P_f = 1 \text{ atm} \\ T_f = 298 \text{ K} \\ T_{ox} = T_2 \end{array} \end{array} \right\}$$

$$\Rightarrow h_4, S_4$$



$$\Phi_{AF} \Rightarrow \dot{m}_a, \dot{m}_f, \dot{m}_p$$

$$\dot{Q}_{comb} = T_0 [\dot{m}_p S_4 - \dot{m}_a S_2 - \dot{m}_f S_3]$$

Note: You can use the air table to get S_2 for $\dot{Q}_{comp}$, but you must use

$$S_2 = \sum n_i S_i$$

where S_i for O_2, N_2 here to keep calc consistent.

Turbine.

a) Not air anymore

b) Gases react as they cool and expand. $[CO \rightarrow CO_2]$

1st Let $S_5 = S_4$ [Pressure down $\Rightarrow$ T down to keep disorder constant]

Code:

$$\left. \begin{array}{l} \text{CH}_4 / \text{air} \mid \Phi_{AF} \text{ from above} \mid \text{TP} \mid \begin{array}{l} P_f = 1 \text{ atm} \\ T_f = \text{guess} \end{array} \end{array} \right\} \text{Iterate on } T_f \text{ until } S_5 = S_4 \Rightarrow h_{5,s}$$

$$\text{Then } \eta_T = \frac{h_4 - h_{5,s}}{h_4 - h_{5,a}} \Rightarrow h_{5,a}$$

Now use code to find other properties @ (5)

$$\left. \begin{array}{l} \frac{\text{CH}_4}{\text{air}} \mid \Phi_{AF} \mid TP \mid \left. \begin{array}{l} P_f = 1 \text{ atm} \\ T_f = \text{guess} \end{array} \right\} \begin{array}{l} \text{Iterate on } T_f \text{ until} \\ h = h_{S,9} \Rightarrow S_S, T_{S,9} \text{ etc.} \end{array} \end{array} \right\}$$

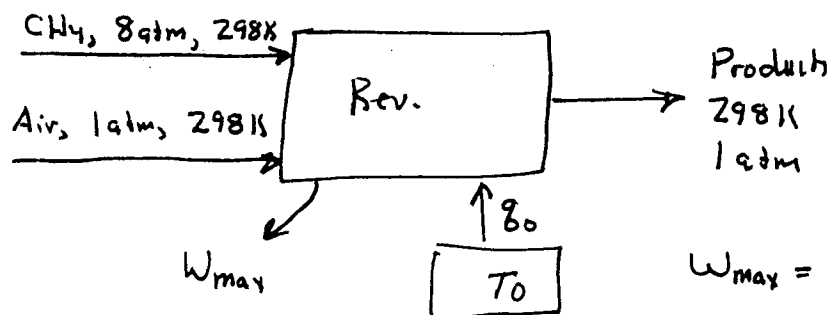
$$\Rightarrow W_T = \dot{m}_P (h_4 - h_5)$$

$$\dot{Q}_T = \dot{m}_P T_0 (S_5 - S_4)$$

Lost Work. $W_{\text{lost}} = \dot{m}_P [h_5 - h_0 - T_0 (S_5 - S_0)]$

$$\left. \begin{array}{l} \frac{\text{CH}_4}{\text{air}} \mid \Phi_{AF} \mid TP \mid \left. \begin{array}{l} P_f = 1 \text{ atm} \\ T_f = 298 \text{ K} \end{array} \right\} \begin{array}{l} h_0 \\ S_0 \end{array} \right\}$$

Finally, original availability.



$$W_{\text{max}} = h_1 - h_0 - T_0 (S_1 - S_0)$$

h_1, S_1 ~~from as~~
from hand calc. as
above

$\Rightarrow$ Watch units and basis!

Results:

Avail	100%
W _{net}	32%
Exhaust	34%
Comb	30%
Comp	2
Turb	2

Compressor?
Exhaust?

Goal of Combined Cycles is to make use of the work potential of this hot exhaust.

Background—

Historically, gas turbine was developed as aircraft power plant
 $\Rightarrow$ light, but very low η .

- 1) Low turbine inlet T
- 2) Bad component η
- 3) Need clean, expensive fuel.

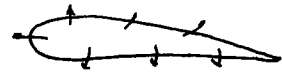
Power generation largely based on Rankine (Coal fuel):

Later, gas turbines got better.

1) Turbine inlet T was improved.

→ Single crystal blades

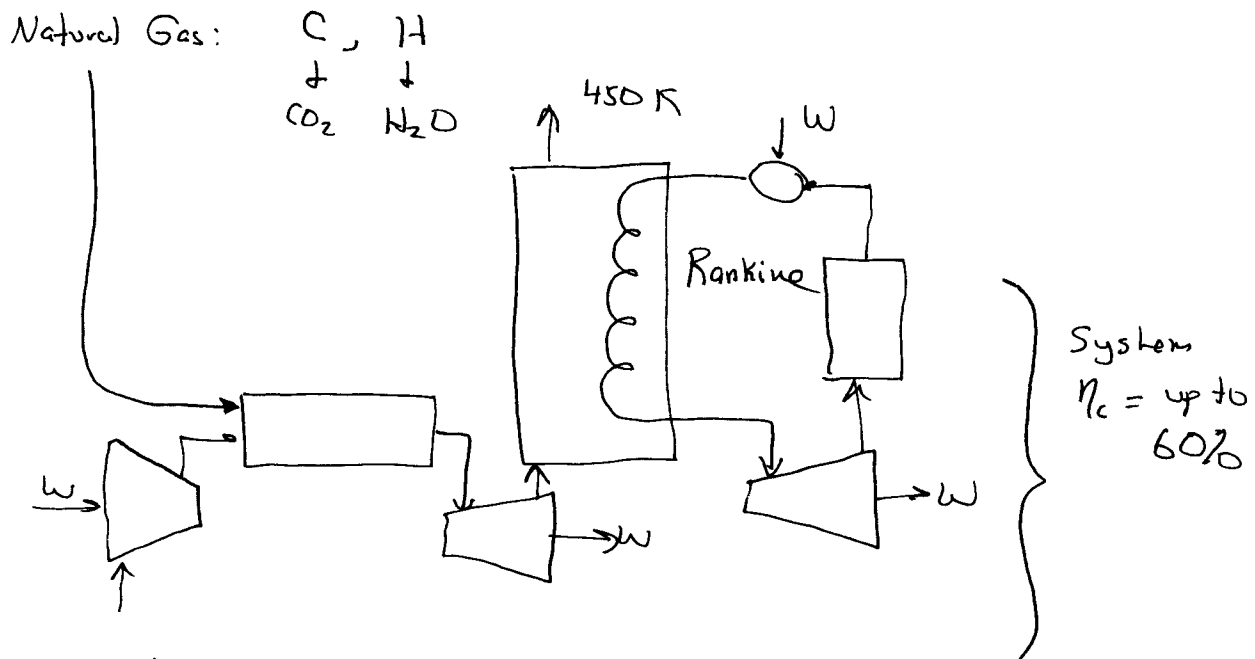
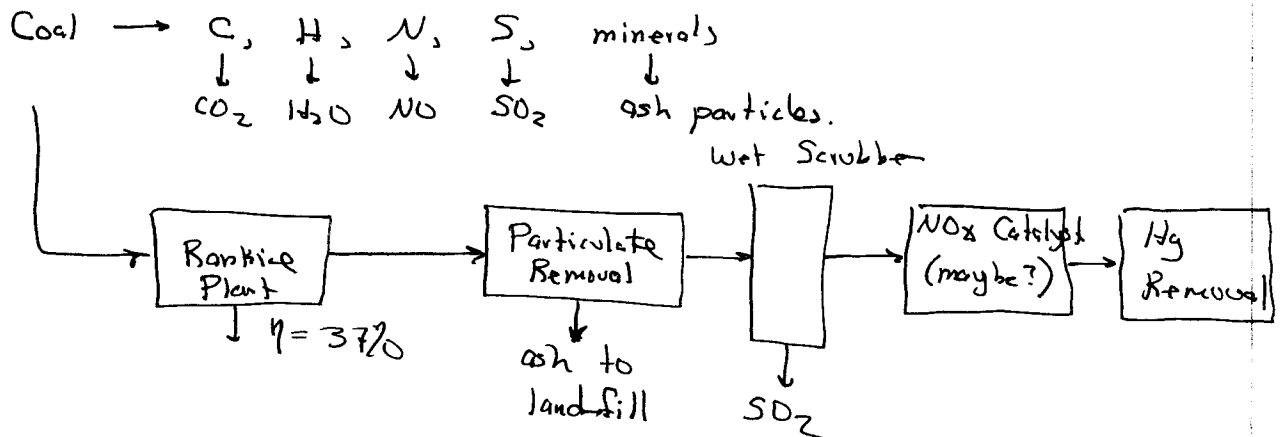
→ Film cooling pushes boundary layer off



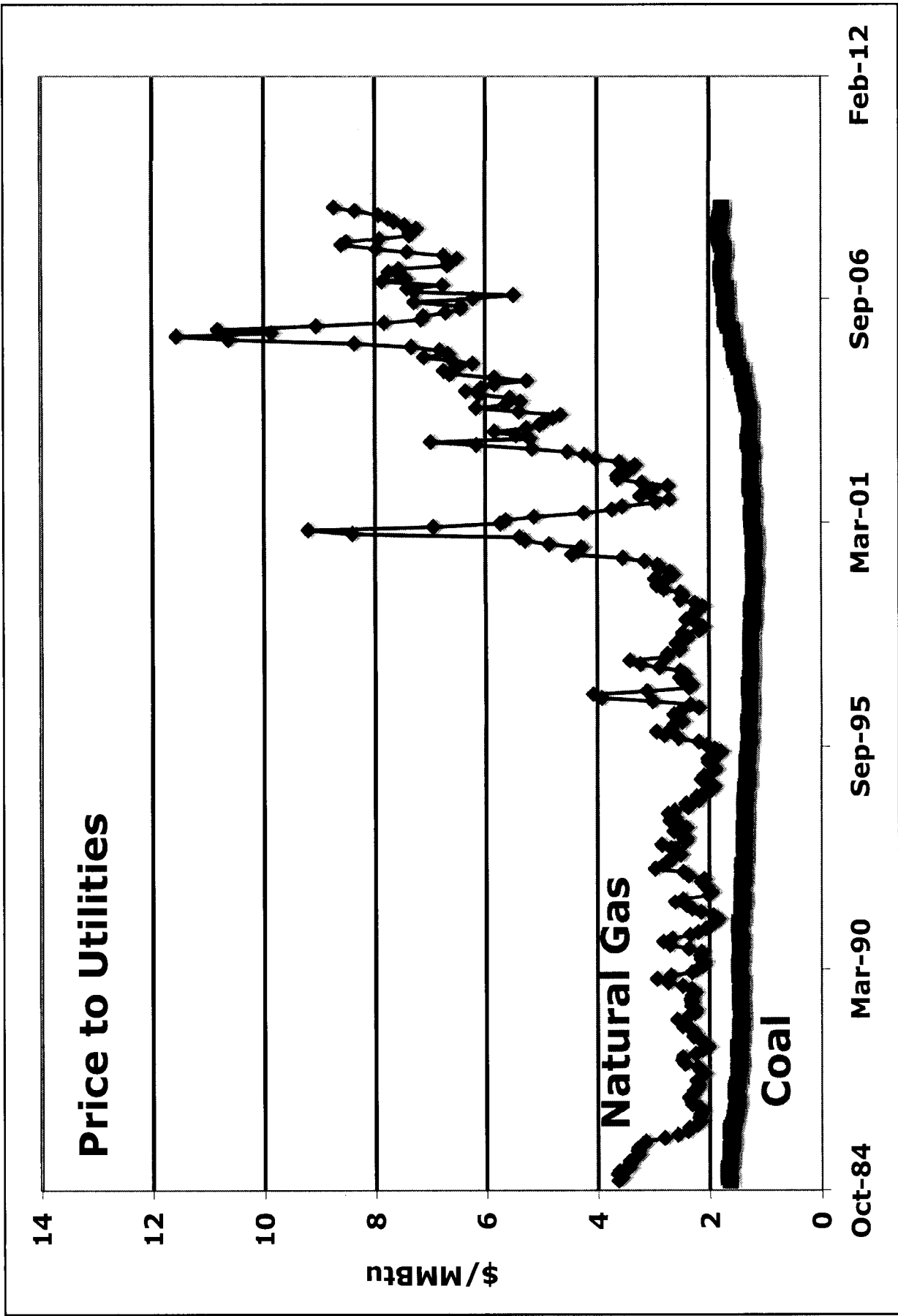
2) Turbomachinery component η improved.

⇒ Direct result of the advent of modern computational fluid dynamics.

So here is the comparison

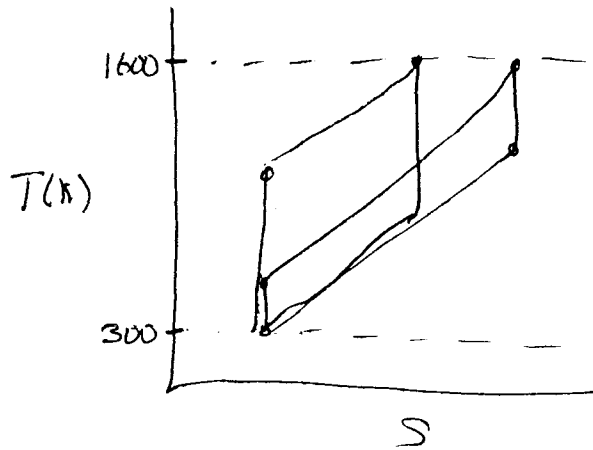


- So can tolerate higher NG costs.
- Since 2000 NG prices have increased and been unstable.
 ⇒ Utilities have had problems attracting investment in new NG-based power systems.



Some design points —

- Simple Brayton used - No regeneration
 → Since hot exhaust is available for Rankine,
 why pay for additional Brayton hardware —
- Main Brayton design point is r_p



- ⇒ Low r_p , hot exhaust.
- ⇒ Too cold, not enough T for Rankine
- ⇒ Too hot, will pick up i in HRSG due to ΔT .
- ⇒ Pick r_p to get good match with steam cycle

⇒ Generally $\sim 800\text{K} \Rightarrow r_p = 20-25$

⇒ Get from aeroderivative engines.

Oct. 10

Rankine Cycle Parameters

- Condenser pressure - low
 - Boiler pressure
 - Superheat T
- } Optimize with r_p .

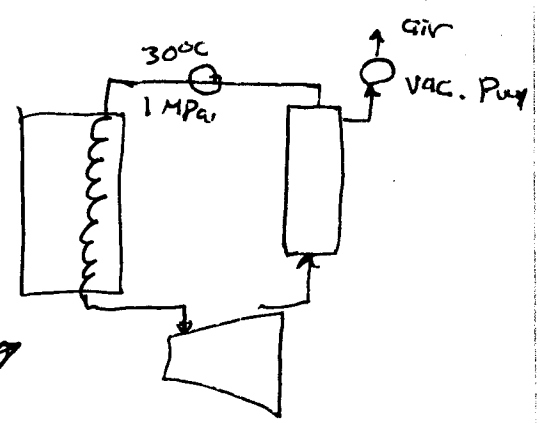
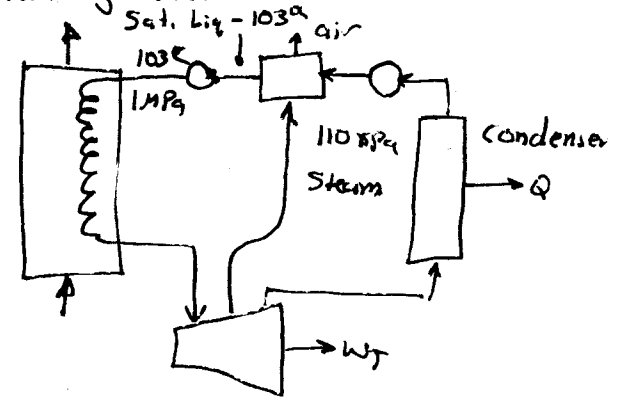
⇒ Simple combined cycle ⇒ r_p (gas turbine exhaust T),
 - P - Boiler
 - Superheat T.

So focus of design is around heat exchanger/boiler.

But: Final point is degeneration - Dissolved O_2 in feedwater & steam is corrosive (< 7 ppm).

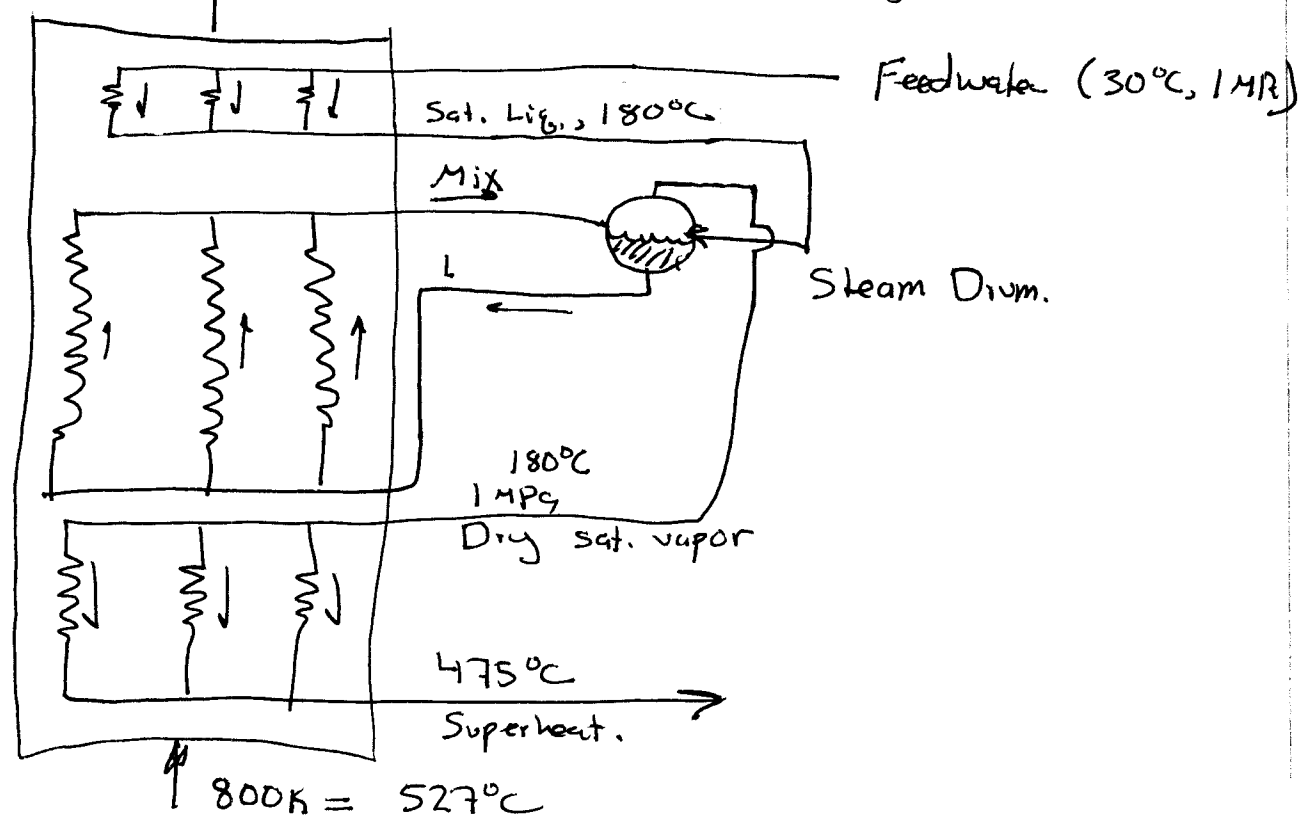
→ From condenser inleakage, startup, makeup water.

① Deaerating feedwater heater.

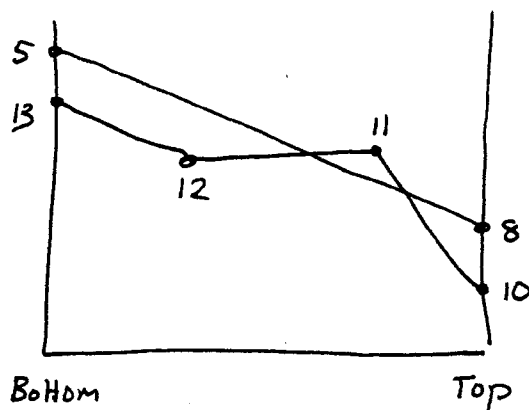
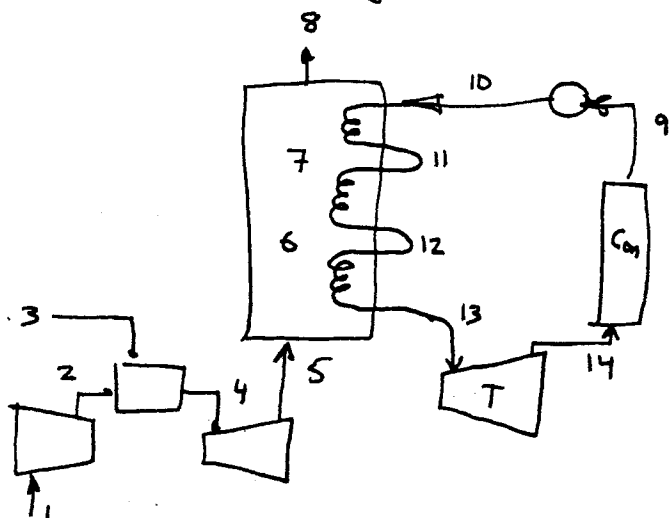


② ~~Condensing~~ Deaerating Condenser

Which would you use?

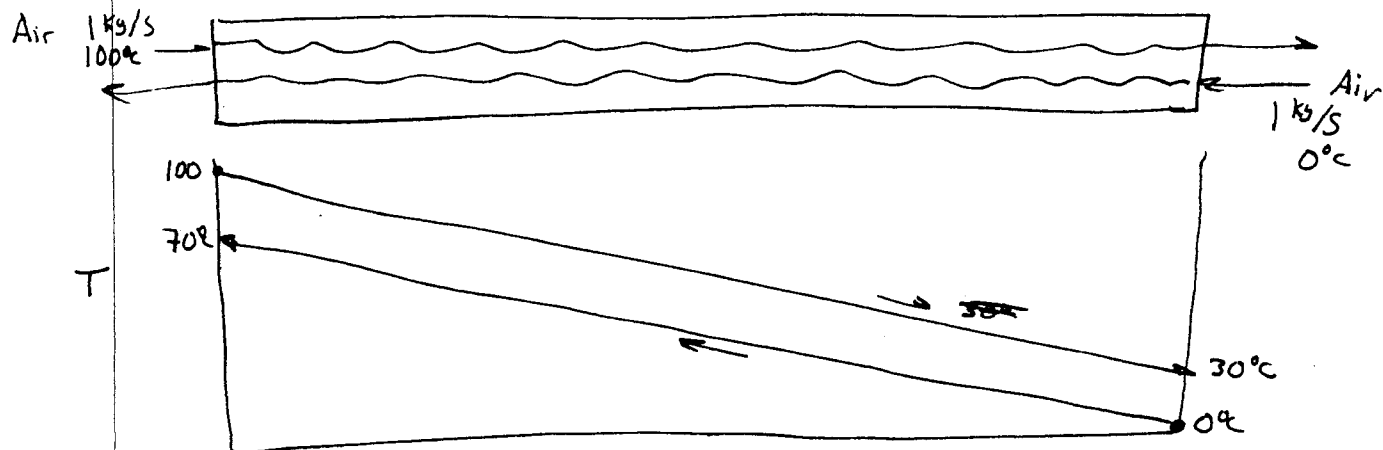


Now to HRSG thermodynamics.

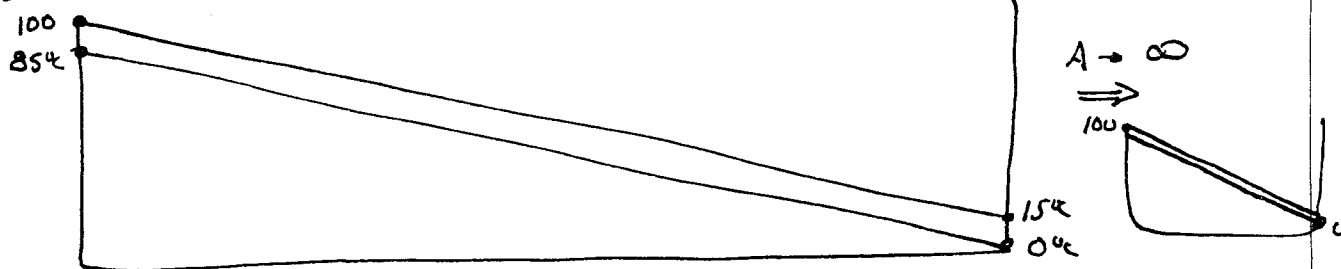


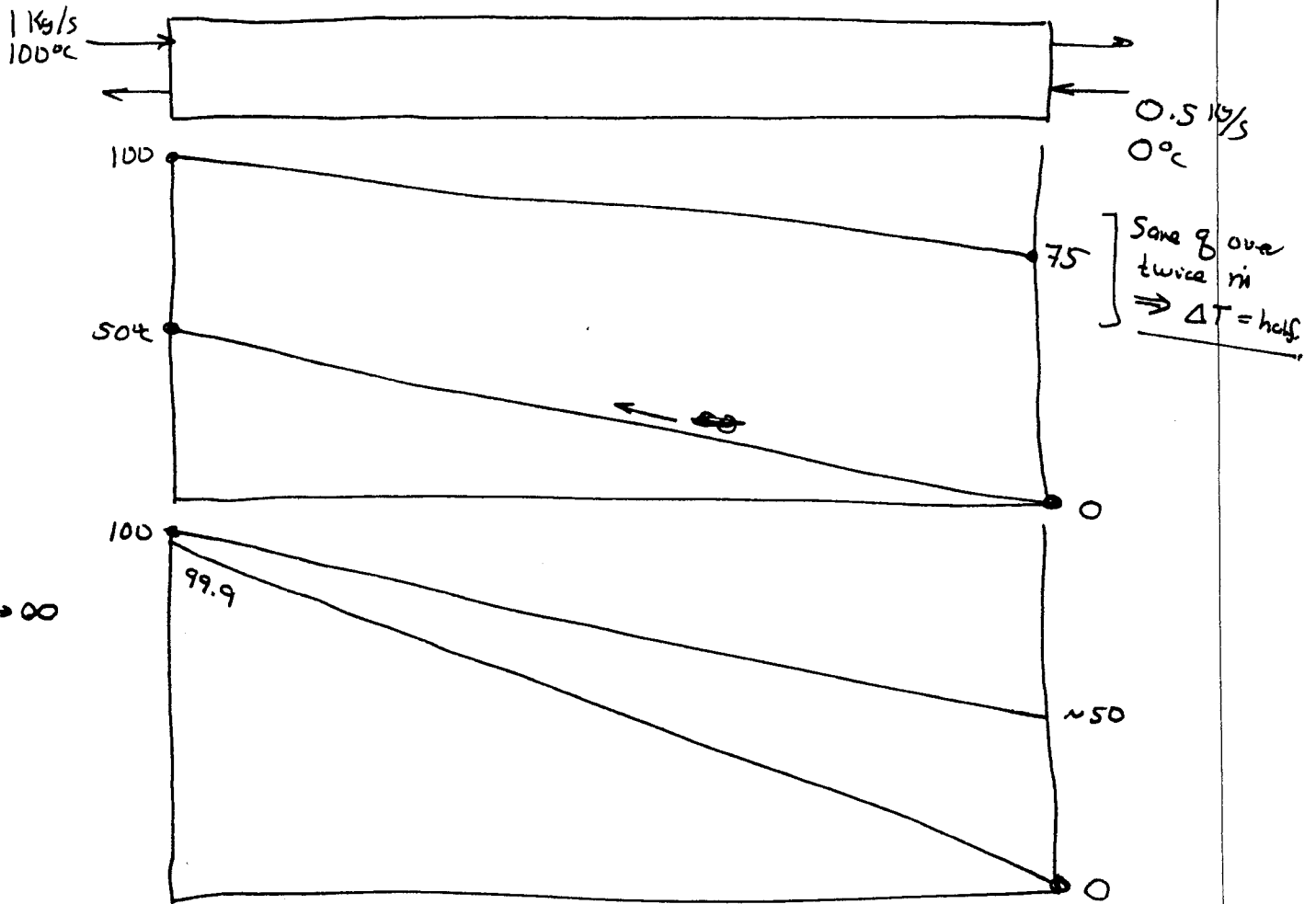
Can have $T_5 > T_{13}$ and $T_8 > T_{10}$ and still have an internal 2nd law violation $\Rightarrow$ "Pinch Point Violation".

Do an aside on HX operation:



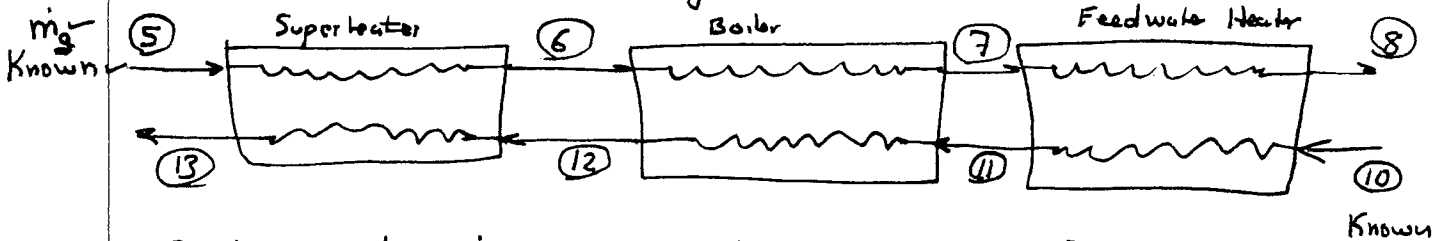
Double Area.





The lower stream has the limiting heat capacity

Now look @ HRSG as a counterflow system.



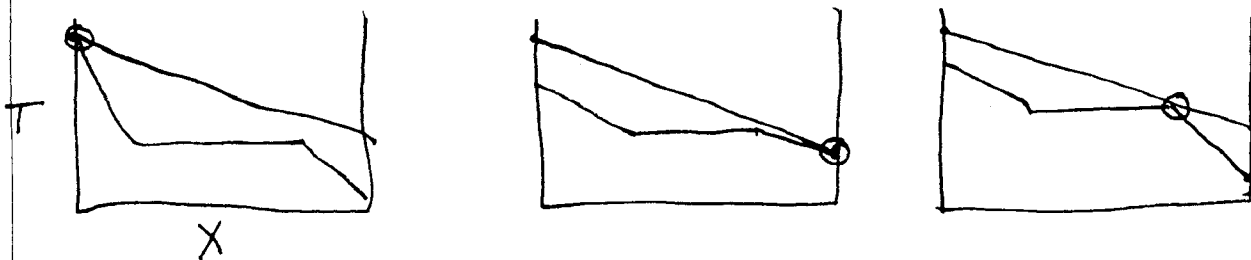
• Brayton provides m_g , T_5 ; T_5 set by r_p = free parameter.

• P_{10} (boiler pressure) a free parameter.

• $T_{13} \leq 620^\circ\text{C}$ due to material constraints.

• $T_{10} = 30-40^\circ\text{C}$

With these choices made, if the HRSG gets arbitrarily large, one of three things will happen.



Oct 11

- We need to detect which limiting case controls:
- Economics $q = h A_s \Delta T \Rightarrow \Delta T \sim \frac{1}{A_s}$ and $i \sim \Delta T$

~~ΔT~~	A_s	ΔT	i (rw)
~~40~~	1	40	4
~~20~~	2	20	2
	4	10	1
	8	5	0.5

At some point, a lot of hardware buys you very little reduction in i .

General rule: $\Delta T = 10^\circ\text{C}$ is good economic choice for contact between gas and condensed phases (boiler, feedwater heater).

For superheater you have gas vs. gas heat exchange $\Rightarrow$ more or less efficient?

$\Rightarrow$ Limiting ΔT higher due to more SA needed.

~~Desio~~ $\Rightarrow$ Rule: $\Delta T = 50^\circ\text{C}$.

- ① Choose superheat T : Lower of $T_{13} = T_5 - 50$
or 620°C - material limit.

Now check to see if controlling point is @ exit or pinch point.

- ② Assume exit controls. $T_8 = T_{10} + 10^\circ\text{C} \Rightarrow h_8$

Get $\dot{m}_{st}$ from 1st Law: $\dot{m}_g (\bar{h}_5 - \bar{h}_8) = \dot{m}_{st} (\bar{h}_{13} - \bar{h}_{10}) \Rightarrow \dot{m}_{st}$

- ③ Check for PP violation: 1st Law on FWH:

$$\dot{m}_g (\bar{h}_7 - \bar{h}_6) = \dot{m}_{st} (\bar{h}_{11} - \bar{h}_{10}) \Rightarrow h_7 \Rightarrow T_7$$

- Now
- $T_7 < T_{11} \rightarrow T_{11} = T_{54t}$, PP violation
 - $T_7 - T_{11} < 10\text{K} \rightarrow$ Uneconomical design
 - $T_7 - T_{11} > 10\text{K} \rightarrow$ OK, you are done.

- ④ If PP is violated, reset limit @ PP:

$$T_7 = T_{11} + 10 \Rightarrow h_7$$

$$1^{\text{st}} \text{ law on boiler/superheater: } \dot{m}_g (\bar{h}_5 - \bar{h}_7) = \dot{m}_{st} (\bar{h}_{13} - \bar{h}_{11})$$

note that $\dot{m}_{st}$ will be smaller than in failed case

- ⑤ Get actual outlet T_8

$$1^{\text{st}} \text{ Law on HRSS: } \dot{m}_g (\bar{h}_5 - \bar{h}_8) = \dot{m}_{st} (\bar{h}_{13} - \bar{h}_{10})$$

$$\Rightarrow h_8 = T_8. \quad \text{will find } T_8 - T_{10} > 10\text{K.}$$

Let's run a numerical example:

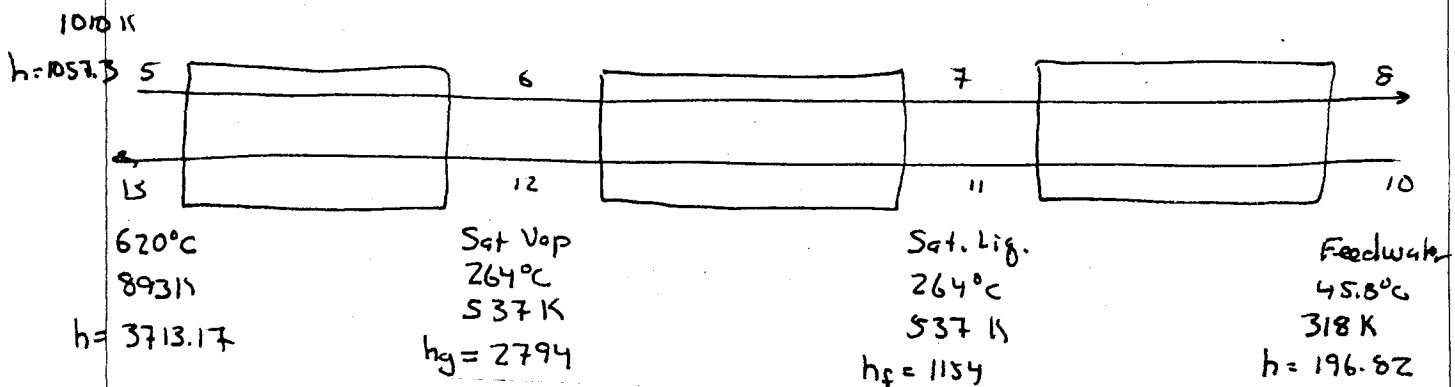
Gas Turbine [variable Cp air analysis, not like your HW].

	T	h
$r_p = 12$	1 300	300.19
$\gamma_c = 0.83$	2 655	655.43
$\eta_T = 0.9$	4 1700	1880.3
$T_1 = 300\text{ K}$	5 1010	1057.3
$T_4 = 1700\text{ K}$		

Steam Cycle

	h	
$P_B = 5\text{ MPa}$	9 191.83	Sat. 10 MPa
$P_C = 10\text{ MPa}$	10 196.82	$h_g + w_p$
$\eta_T = 0.78$	11 1154.0	Sat. Lig. 5 MPa
$T_{13} = 620^\circ\text{C}$	12 2794.0	Sat. Vap. 5 MPa
	13 3713.17	620°C 5 MPa
	14 2623.78	Isentropic to 10 MPa + η_T

Paste info on diagram:



Chose basis 1 kg air

$$\text{Let } T_8 = T_{10} + 10 = 328\text{ K} \Rightarrow h_8 = 328.3\text{ kJ/kg}$$

$$\text{Now get } \dot{m}_s : \dot{m}_g (h_5 - h_8) = \dot{m}_s (h_{13} - h_{10})$$

$$[1][1057.3 - 328.3] = \dot{m}_s [3713.17 - 196.82] \Rightarrow \dot{m}_s = 0.207\text{ kg/s}$$

Now check PP: 1st Law on either boiler + super or FWH

$$\dot{m}_g [h_2 - h_8] = \dot{m}_s [h_{11} - h_{10}] \Rightarrow [1][h_2 - 328.3] = [0.207][1154 - 196.82]$$

$$\Rightarrow h_2 = 526.44\text{ kJ/kg} \Rightarrow T_2 = 577.71\text{ K} \Rightarrow 304.56^\circ\text{C}$$

$\Rightarrow$ This violates PP, so scrap calc and assume new limiting point.

$$T_7 = T_{11} + 10 = 547\text{ K} \Rightarrow h_7 = 552.32\text{ kJ/kg}$$

$$\text{Get } \dot{m}_s : \dot{m}_g (h_5 - h_7) = \dot{m}_s (h_{13} - h_{11})$$

$$[1][1057.3 - 552.32] = \dot{m}_s [3713.17 - 1154] \Rightarrow \dot{m}_s = 0.197\text{ kg/s}$$

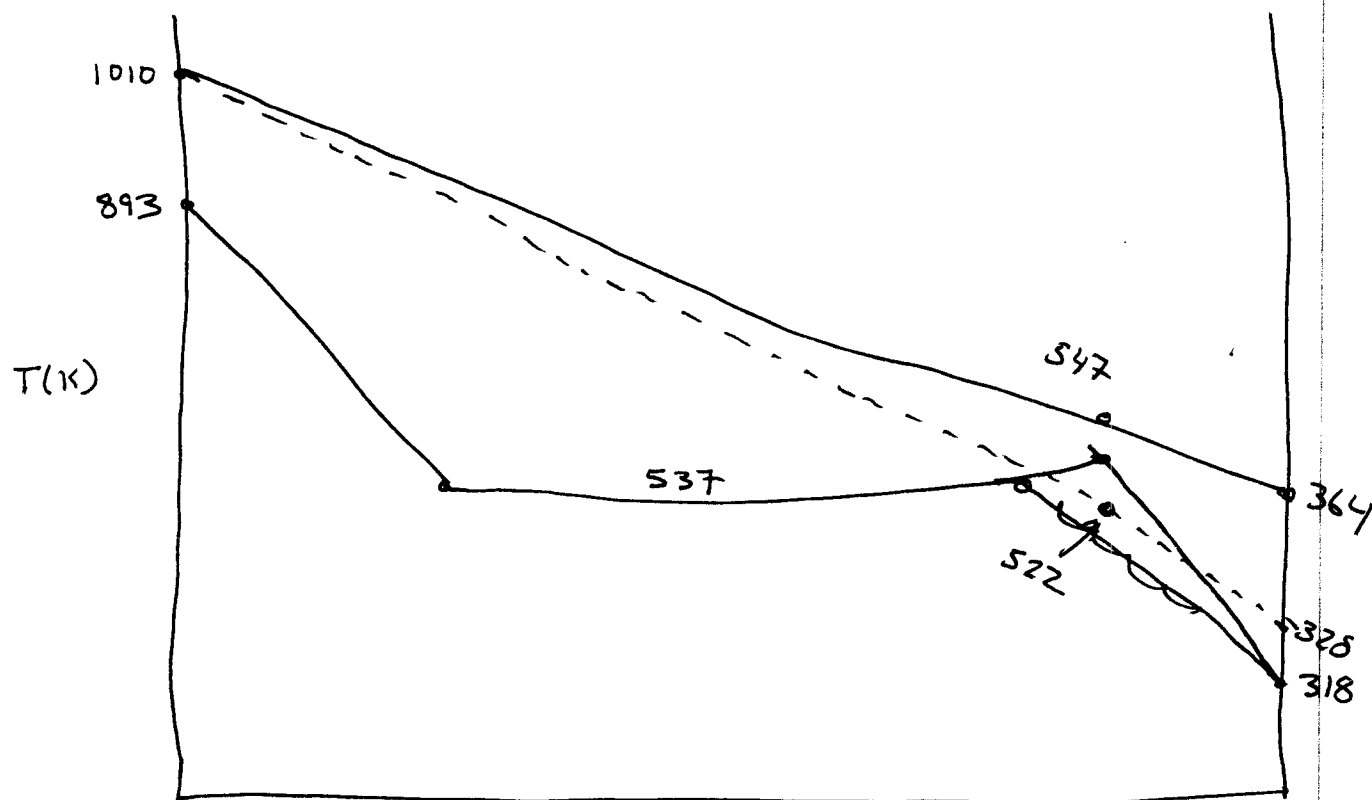
Oct 12

Now T_8 : $\dot{m}_g (h_5 - h_8) = \dot{m}_{st} (h_{13} - h_{10})$

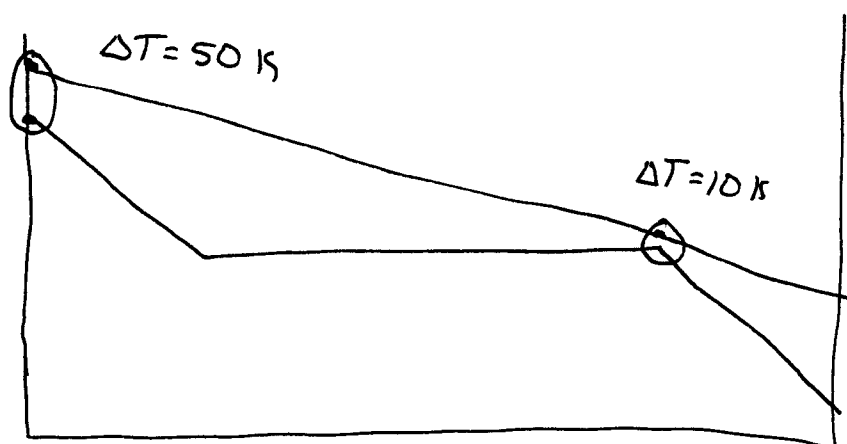
(1) $(1057.3 - h_8) = [0.197][3713.2 - 196.82]$

$\Rightarrow h_8 = 364.6 \text{ kJ/kg}$

$\Rightarrow T_8 = 364 \text{ K} = 91^\circ\text{C}$

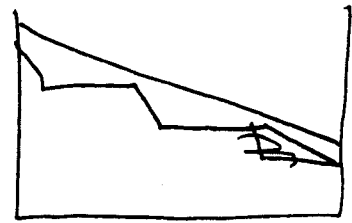


Best performance?



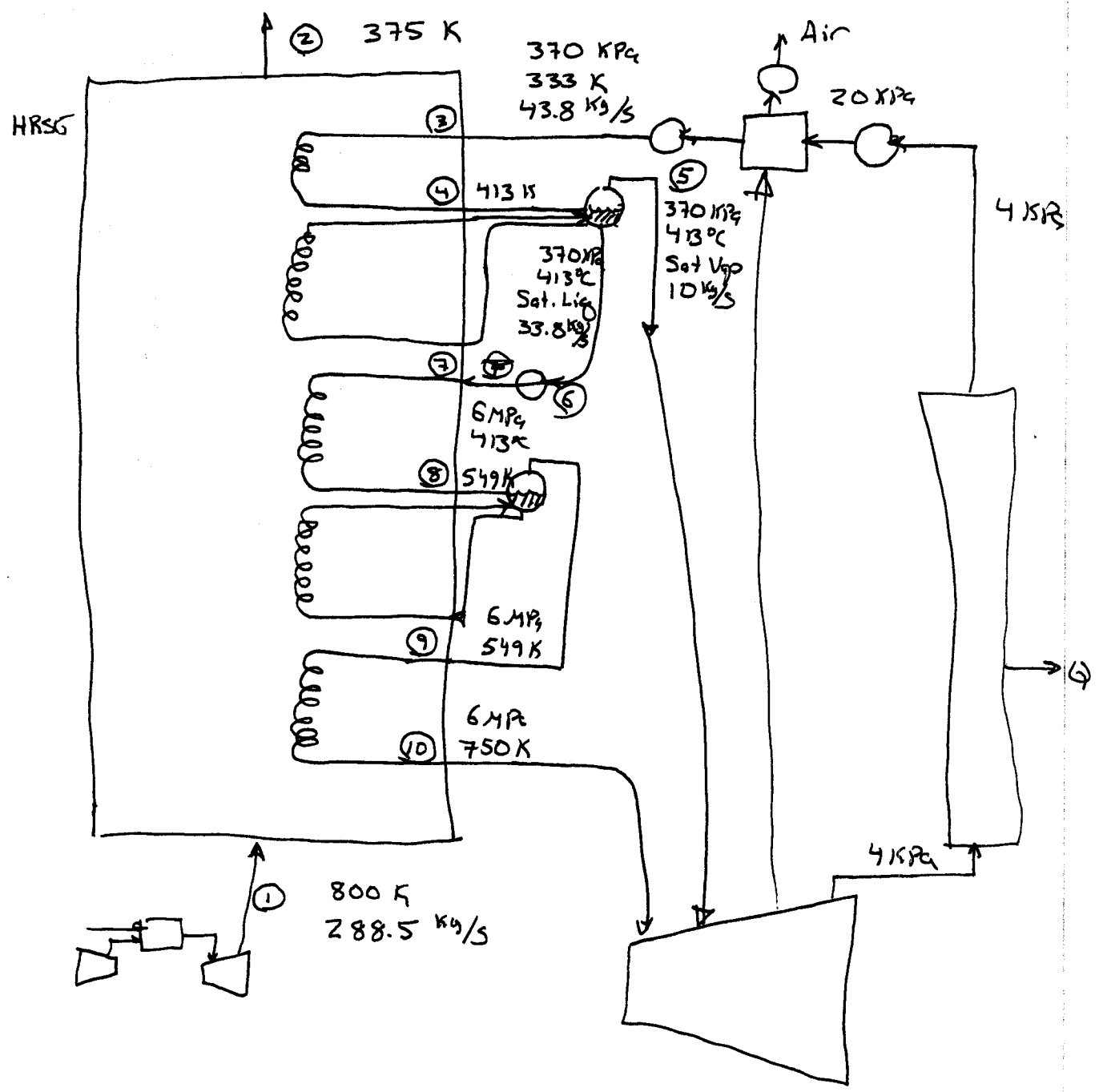
Ends up that boiler P , T -superheat not critical to overall cycle η . Lower superheat $\Rightarrow$ move r_p to keep $\Delta T = 50^\circ\text{C}$.

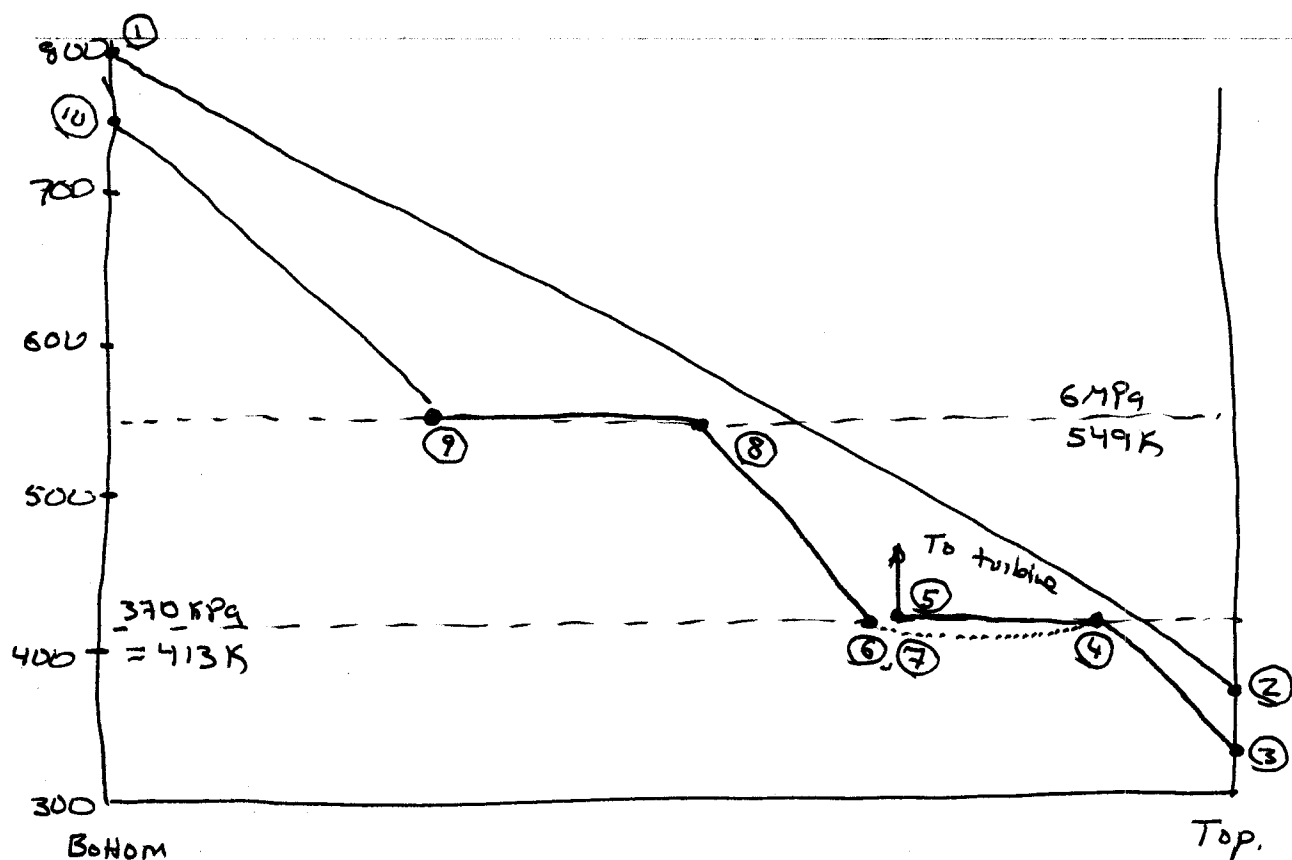
How to do better? Multi-pressure system achieves stair-step effect.



⇒ But it is a little tricky!

Look at actual two-pressure system:





- 3-4 $\Rightarrow$ All water heated to saturation
 4-5 $\Rightarrow$ 10 kg/s is boiled and sent to turbine
 4-6 ~~5-6~~ $\Rightarrow$ 33.8 kg/s kept as liquid and bypassed
 6-7-10 $\Rightarrow$ Pump to 6 MPa, boiled, and superheated

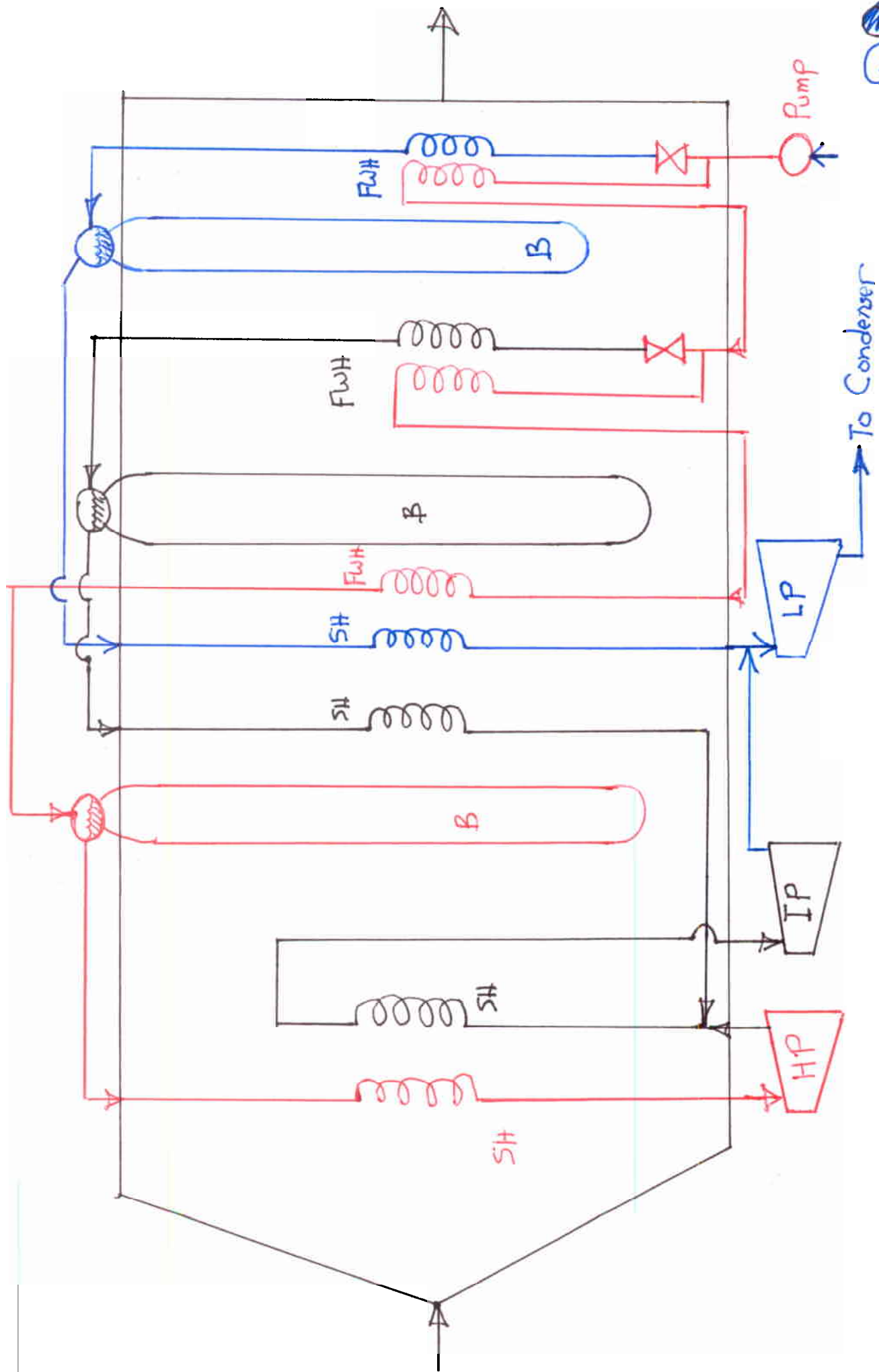
Compare to single-pressure system. (6 MPa)

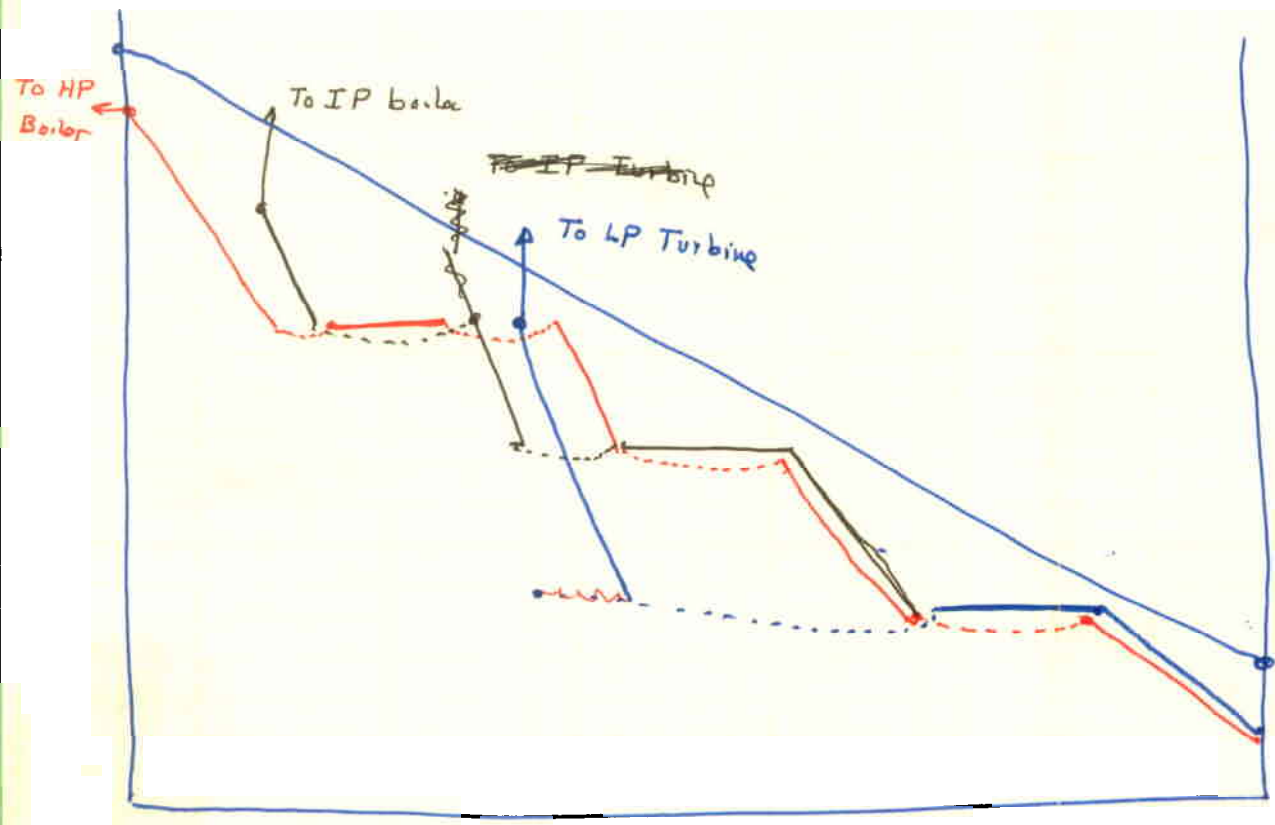
- $\Rightarrow$ Pinch point becomes limit
 $\Rightarrow$ Steam flow reduced to 35.3 kg/s
 $W_{\text{net}} \quad 40.8 \rightarrow 33.1 \text{ MW}$
 $\Rightarrow T_2$ rises ~~to~~ from 375 K to 438 K.

Now look briefly at GE class H system (highest η_c on market)

$\eta_c = 60\%$ on fuel LHV = 800,800 kJ/kmole
 $\Rightarrow W_{\text{net}} = 480,480$

Remember that $W_{\text{max}} = 576,000$ for comb + heat engine
 $\Rightarrow$ 83% recovery for this system.





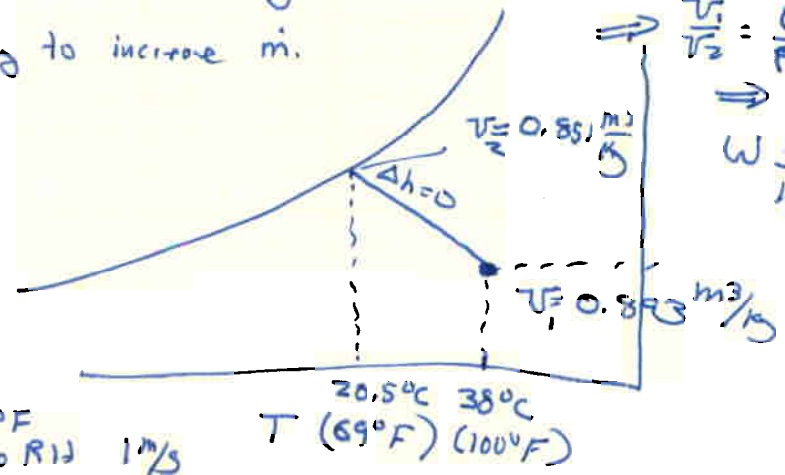
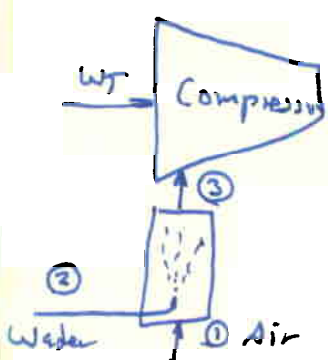
Other features:

- Steam cooling of gas turbine blades
 $\Rightarrow$ Recover heat for steam cycle
- Single crystal turbine blades
- Use steam preheat on fuel
- Deaerating condenser.
- Corrosion-resistant low-T feedwater tubes
- Air intake cooling $\Rightarrow$

$$\frac{P_{100^\circ F}}{P_{30^\circ F}} = 0.875$$

Since ~~turbine~~ compressors are volume ~~compressors~~ hot day really reduces what you can process

Use evaporative cooling to increase $\dot{m}$.



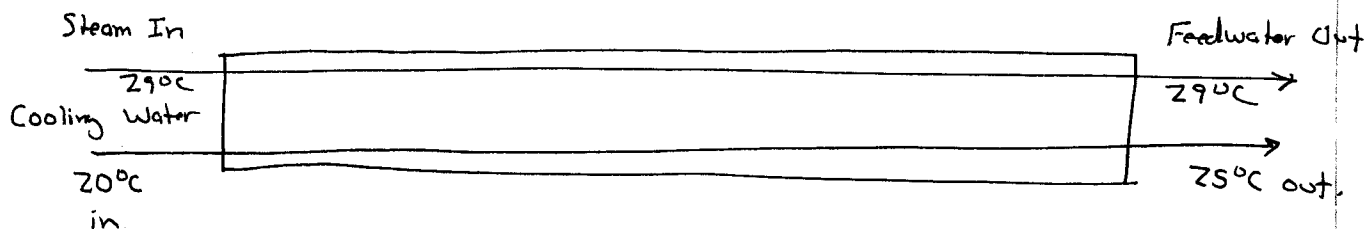
$$\Rightarrow \frac{V_1}{V_2} = \frac{P_2}{P_1} = 1.05$$

$\Rightarrow$ 5% increase in power,
W $\frac{H_2O}{15 \text{ dry air}}$

Oct. 15

Condenser Pressure = 4.1 kPa = 29°C = 84°F
⇒ On hot day may need to derate system.

Look at size 400 MWe out @ 60% eff ⇒ 667 MW fuel in
⇒ $\dot{Q}_{out} = 267 \text{ MW}$.



Mass of Water? 1st Law on bottom half of exchanger.

$$\dot{Q} = \dot{m}_w C_{p,w} (\Delta T)$$
$$267,000 \text{ kJ/s} = (\dot{m}_w) (4.184 \text{ kJ/kg H}_2\text{O-K}) (5 \text{ K}) \Rightarrow 12,800 \text{ K/s}$$
$$\Rightarrow 12.8 \text{ metric tons/s}$$

⇒ Either on a large body of water, or you need cooling towers.

Also look at size of condenser:

$$\dot{Q} = h A_s \Delta T$$
$$267,000 \frac{\text{kJ}}{\text{s}} = \left[700 - 10,000 \frac{\text{J}}{\text{s-m}^2-\text{K}} \right] \left[10^{-3} \frac{\text{kJ}}{\text{J}} \right] A_s [29 - 22.5 \text{ K}]$$
$$\Rightarrow \frac{\text{ft} \times \text{ft}}{800 \times 800 \text{ ft}} \Rightarrow \frac{\text{ft} \times \text{ft}}{210 \times 210 \text{ ft}}$$
$$A_s = 59,000 \text{ m}^2$$
$$= 4100 \text{ m}^2$$

Economics. Unit cost ~ \$500/kW, 30 year life, $\eta_c = 58\%$, 80% Capacity Factor.
NG = 8\$/10⁶ Btu delivered. 6% interest, 400 MW.

$$\frac{\text{Fuel Cost}}{\text{yr}} = \frac{400,000 \text{ kW} \cdot \text{yr}}{\text{s}} \cdot \frac{\text{kJ}}{\text{m}} \cdot \frac{0.948 \text{ Btu}}{\text{kJ}} \cdot \frac{8 \$}{10^6 \text{ Btu}} \cdot \frac{0.8}{\text{yr}} = 131.8 \text{ E}+6 \text{ \$/yr}$$

$$\text{Capital Cost: } \frac{\$500}{\text{KW}} \cdot 400,000 \text{ KW} = 200. \text{ E}+6 \$$$

Capital recovery factor - \$/yr ~~needed~~ including interest, needed to wipe out debt in 30 yrs

$$\frac{A}{P} = \frac{i}{1 + (1+i)^{-n}} = \frac{0.06}{1 - (1+0.06)^{-30}} = 0.0726$$

$$\text{Annual cost of capital: } [0.0726] [200 \text{ E}+6] = 14.5 \text{ E}+6 \text{ \$/yr.}$$

$$\text{Total cost: } 131.8 \text{ E}+6 + 14.5 \text{ E}+6 = 146.3 \text{ E}+6 \text{ \$/yr.}$$

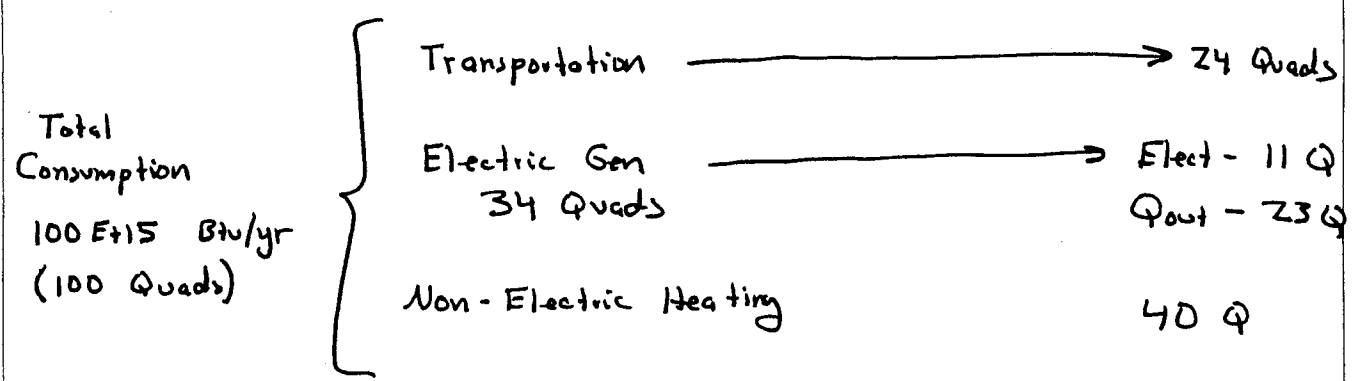
(90% Gas) (10% Capital)

$$\frac{\$/\text{KW-hr} ?}{\text{yr}} = \frac{146.3 \text{ E}+6 \$}{\text{yr}} \cdot \frac{\text{yr}}{400,000 \text{ KW} \cdot 0.8 \cdot 8760 \text{ hr}} \Rightarrow 5.22 \text{ \$/KW-hr}$$

(1.99¢ for 2.5 \$/10⁶ Btu gas).
So gas costs an issue —

Oct 17

Very briefly summarize US energy picture.

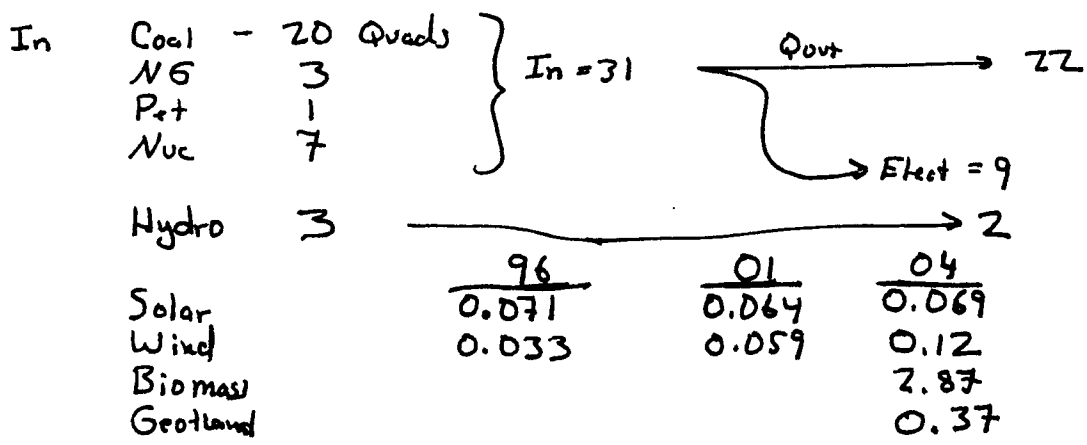


Put into perspective: 330 E+6 Btu/yr-capita → 2400 gal/day yr
or 6.5 gal/day.

Look at via resource:

	Trans	Elect	Heating
Coal: 24 Q Dug		20 Q (rest to coke, export)	
NG 22 Q	1 Q	3 Q	18 Q 11 - Ind 4 - Res 3 - Comm
Petroleum 21 Imp 16 Dom	24 Q	1 Q	12 Q 9 - Ind 3 - Res
Nuclear		7 Q	
Hydro		3 Q	

Electricity.



Coal is source of about 60% of US Electricity.

Look @ how much

$$\frac{20 \text{ EJ} + 15 \text{ Btu}}{\text{yr}} \left| \frac{\text{KJ}}{0.946 \text{ Btu}} \right| \left| \frac{\text{MJ}}{10^3 \text{ KJ}} \right| \left| \frac{\text{kg}}{30 \text{ MJ}} \right| \left| \frac{\text{m}^3}{1200 \text{ kg}} \right| \Rightarrow \text{Cube } 837 \text{ m on a side.}$$

We each are responsible for $\sim 2.3 \text{ tons/yr}$ or cube 1.25 m on side
 $\Rightarrow 16 \text{ kg CO}_2 \text{ day.}$

- Coal: • Basically fossilized ^{organic} ~~matter~~ matter
 • Collected anaerobically in swamps.
 • Compressed, aged.
 • Classes
- Peat
 - Lignite (West US)
 - Bituminous (Most US)
 - Anthracite $\rightarrow$ almost graphite (little)
- ↓
Older

Consists of organic matter C, H, O, N, S
 + minerals (Al, Fe, Si, Na, Ca, Mg, etc.) Like Earth's crust.

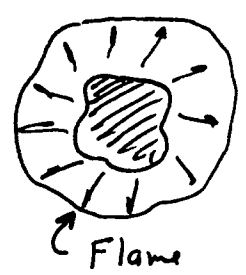
Ship in unit trains $\Rightarrow$ 600 MWe plant

$$\frac{600 \text{ MJe}}{\text{s}} \left| \frac{\text{MJm}}{0.37 \text{ MJe}} \right| \left| \frac{\text{kg}}{30 \text{ MJ}} \right| \left| \frac{3600 \text{ s}}{\text{hr}} \right| \left| \frac{24 \text{ hr}}{\text{d}} \right| \Rightarrow \sim 4500 \text{ tons/day}$$

$\sim 45 \text{ } 100 \text{ ton}$
carloads.

Grind to 50-70 μm for burning. (hair thickness).

The combustion process: (like a charcoal briquette).



Devolatilization
~ 20 ms.

1. Radiation from flame heats coal
2. Coal breaks down
 $\Rightarrow$ $\text{CO}, \text{H}_2\text{O}, \text{H}_2, \text{CH}_4$ off
 $\Rightarrow$ Left behind is C.



Char
Combustion
~ 0.5 s

↓
Sets size
of furnace.

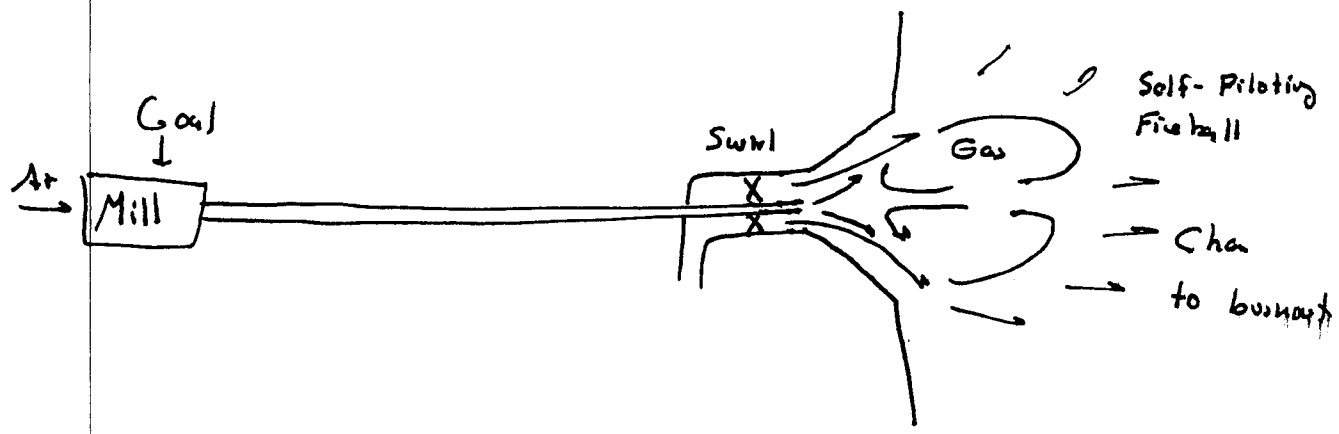
3. When all gases are gone, get direct C + O_2 combustion @ surface.
 $\rightarrow$ Glowing briquette stage.
 $\rightarrow$ Briquettes are white because of mineral



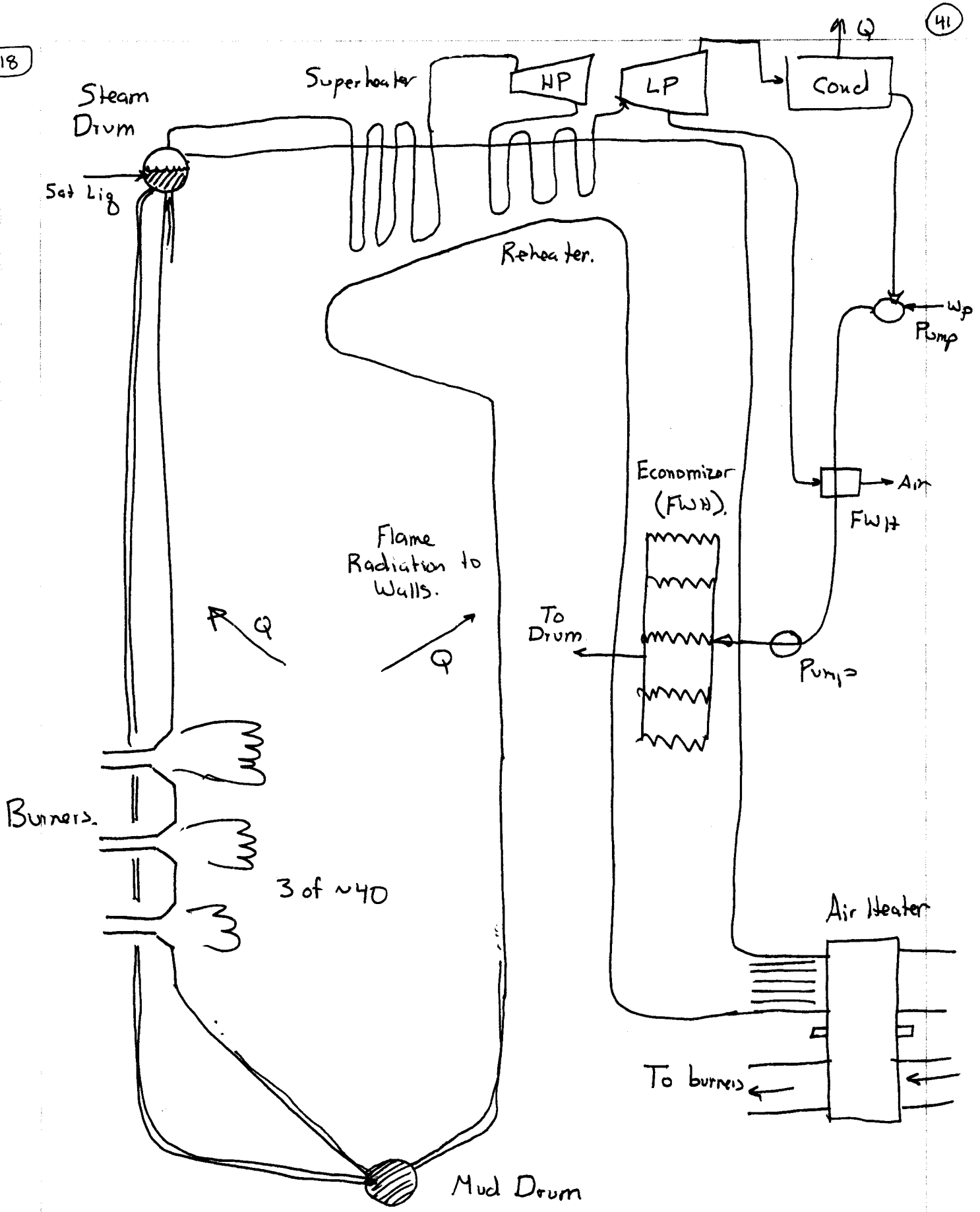
4. When carbon is burned out remaining mineral cokes into ash particles.

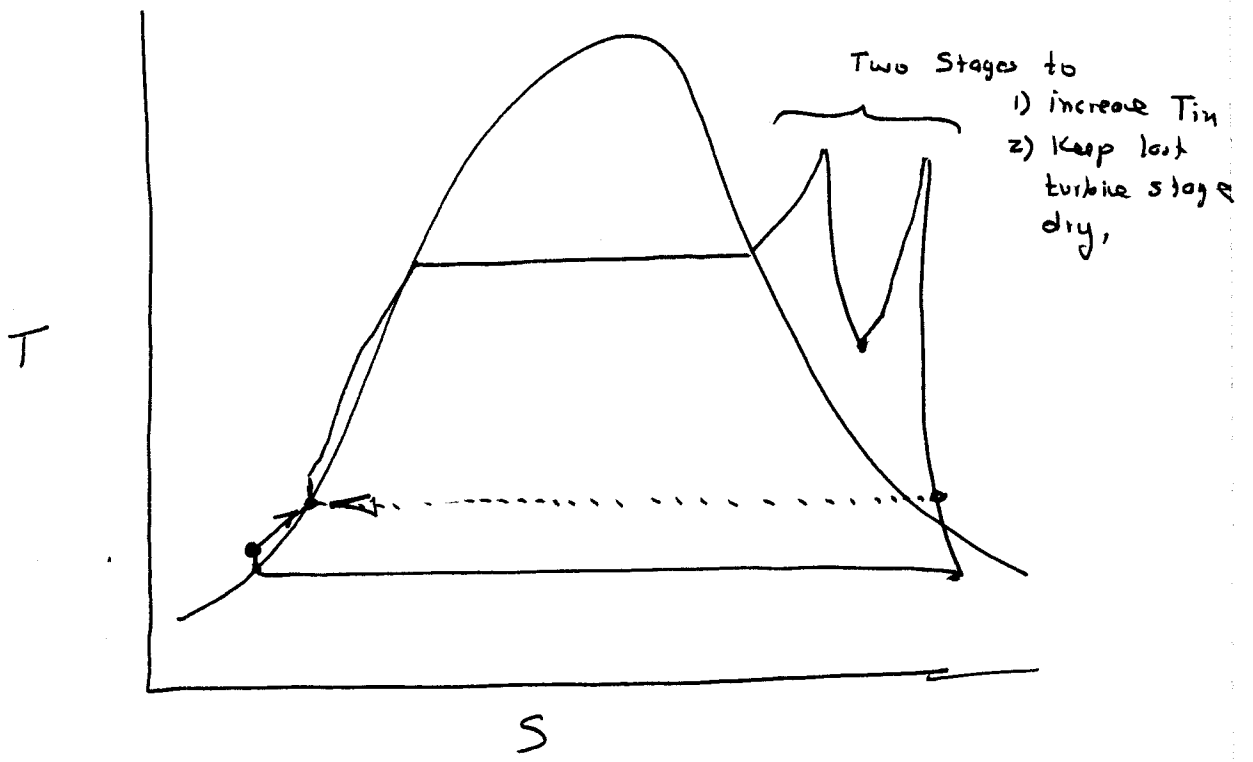
$\text{Al}_2\text{O}_3, \text{FeO}_2, \text{CaO}, \text{SiO}_2$, etc.

Most common combustion technology is Wall-Fired.



Oct 18

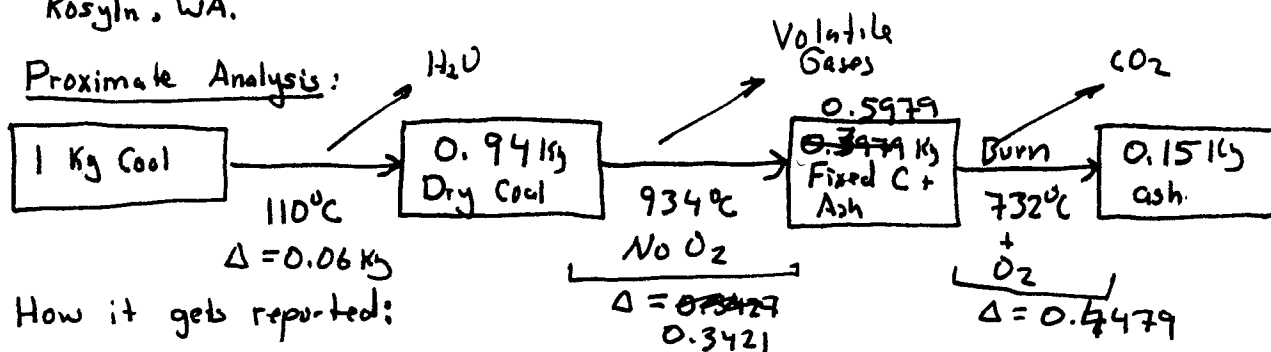




Coal Analysis - A nomenclature of its own.

Roslyn, WA.

Proximate Analysis:



How it gets reported:

$$\text{Ash} = \frac{0.15 \text{ kg}}{1 \text{ kg}} = 15\% \text{ Ash}$$

$$\text{Moisture} = \frac{0.06 \text{ kg}}{1 \text{ kg}} = 6\% \text{ Moisture}$$

$$\left. \begin{array}{l} 15\% \text{ Ash} \\ 6\% \text{ Moisture} \end{array} \right\} \text{As received basis}$$

Dry, Ash-Free Coal: $1 - 0.06 - 0.15 = 0.79 \text{ kg DAF}$

$$\left. \begin{array}{l} \text{Volatile Matter: } \frac{0.3421 \text{ kg}}{0.79 \text{ kg}} = 43.3\% \text{ VM} \\ \text{Fixed Carbon: } \frac{0.4479 \text{ kg}}{0.79 \text{ kg}} = 56.7\% \text{ FC} \end{array} \right\} \text{DAF Basis}$$

Why? H_2O and Ash vary a lot within mine (where, how much earth included).
VM and FC relatively fixed when you get "dilvents" out.

Proximate gives ① Burning characteristics (VM gives stable flames),
② Rank. (VM down as rank goes up).

"Approximate" analysis.

Ultimate Analysis.

	% DAF	0.79 kg DAF mass	Kmols
C	80.5	0.636	$5.30 \text{ E-}2$
H	6.0	0.0474	$4.74 \text{ E-}2$
O	10.8	0.0853	$5.33 \text{ E-}3$
N	1.9	0.0150	$1.07 \text{ E-}3$
S	0.8	0.0063	$1.97 \text{ E-}4$
		0.790	

HHV = 34,005 kJ/kg DAF

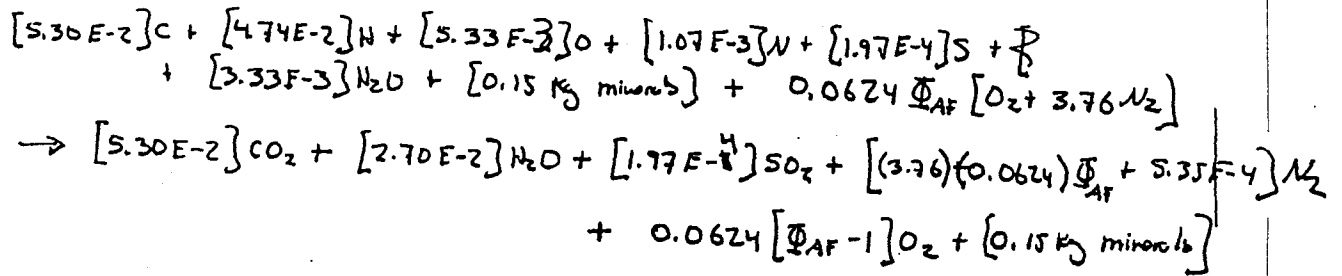
$\text{H}_2\text{O} = 0.06 \text{ kg} = 3.33 \text{ E-}3 \text{ kmols}$

$$[5.3 \text{ E-}2] \text{C} + [4.74 \text{ E-}2] \text{H} + [5.33 \text{ E-}3] \text{O} + [1.07 \text{ E-}3] \text{N} + [1.97 \text{ E-}4] \text{S} + [3.33 \text{ E-}3] \text{H}_2\text{O} + [0.15 \text{ kg minerals}] + W [\text{O}_2 + 3.76 \text{ N}_2] \rightarrow \text{products}$$

$$[5.30 \text{ E-}2] \text{CO}_2 + \frac{[4.72 \text{ E-}2] + [3.33 \text{ E-}3]}{2} \text{H}_2\text{O} + [1.97 \text{ E-}4] \text{SO}_2 + [3.76W + \frac{1.07 \text{ E-}3}{2}] \text{N}_2 + [0.15 \text{ kg minerals}]$$

O-atom:

$$5.33 \text{ E-}3 + 3.33 \text{ E-}3 + 2W = 2[5.3 \text{ E-}2] + 2.7 \text{ E-}2 + [1.97 \text{ E-}4]2 \Rightarrow W = 0.0624$$



Look at some of the numbers associated with a 600 MWe plant [Seattle averages $\sim \frac{1200}{1000}$ MWe]

$$\frac{600,000 \text{ KJ}_e}{s} \mid \frac{KJ_{in}}{s} \mid \frac{KJ \text{ DAF}}{s} \mid \frac{Raw}{0.79 \text{ KJ DAF}} = 60.36 \text{ kg/s}$$

$\Rightarrow$ 5200 metric tons/day. (train of ~~50~~ 52 = 100 ton

$\Rightarrow$ Ash production = 15% of this $\Rightarrow$ 780 ^{tons/day} ton/day.

Air requirement: $\sim 20\%$ excess air

$$\frac{[0.0624][1.2][32 + 3.76(28)] \text{ kg air}}{\text{kg Raw coal}} = 10.28$$

$$\text{Air Flow: } \frac{60.36 \text{ kg/s} \mid 10.28 \text{ kg Air}}{s \mid \text{kg fuel}} = \frac{620.5 \text{ kg/s}}{534 \text{ m}^3/s}$$

Typical pressure loss $\approx 10''$ water column = 2.8 KPa

$$\dot{W} \equiv \dot{VDP} = \left[534 \frac{\text{m}^3}{s} \right] [2.8 \text{ KPa}] = \underline{1.5 \text{ MW}} \quad [\sim 0.5 \text{ MW/yr}]$$

SO₂ emissions:

$$\frac{60.36 \text{ kg Raw}}{s} \mid \frac{0.79 \text{ kg DAF}}{\text{kg Raw}} \mid \frac{0.008 \text{ kg S}}{\text{kg DAF}} \mid \frac{64 \text{ kg SO}_2}{32 \text{ kg S}} \mid \frac{31.5E+6 \text{ S}}{\text{yr}}$$

$$= 24,000 \text{ tons/yr.}$$

If 6% S $\Rightarrow$ 180,000 t/yr $\Rightarrow$ So a lot of SO₂ control can be achieved by coal choice.

Environmental Issues

- NO_x
- SO_y
- Reactive Hydrocarbons

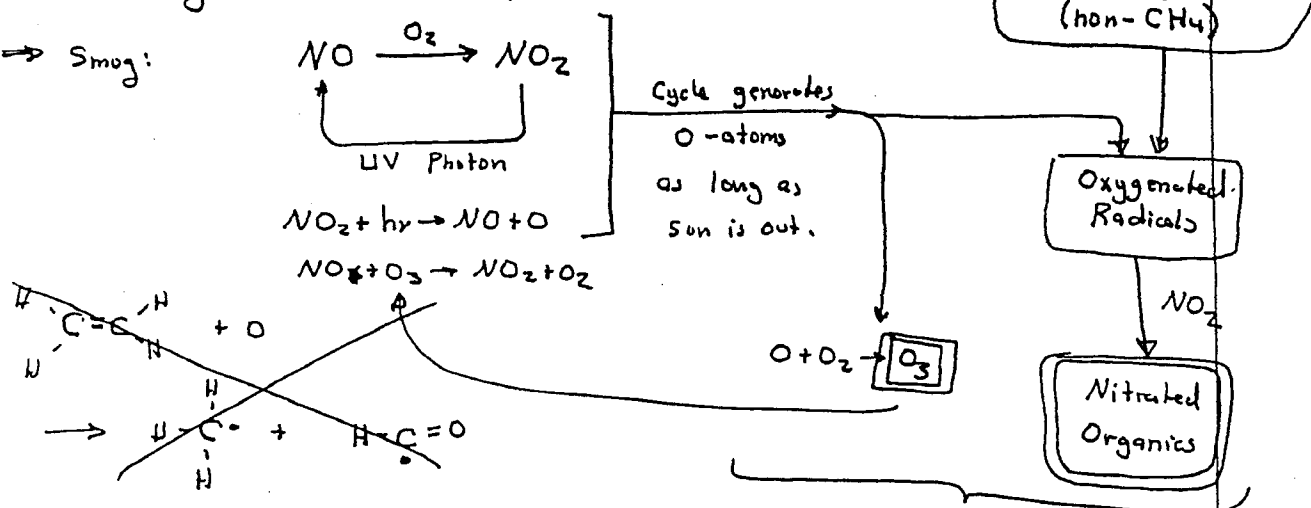
- Particulate matter
- Air Toxics
- Greenhouse Gases.

- Effect
- Where they
- How to control

NO_x : NO : Clear gas, toxicity unclear since it goes to NO_2 in atm.
 NO_2 : Red-brown gas, Cl_2 smell, ambient ≤ 0.5 ppm,
 Lung impacts @ 5-10 ppm.
 $\Rightarrow$ This is what makes smog brown, but it really doesn't have any direct impact.

$\Rightarrow$ Secondary reactions are the problem:

$\Rightarrow$ Smog:



More complicated than shown here.

So you need:

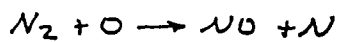
- Sun for photons
- Heat to speed reactions
- NO to make O-atoms
- Hydrocarbons to make nitrated organics.

Good news is that the bad stuff has a short half-life.

- $\rightarrow$ Shut photons off and O_3 /organics are gone in ~ 1 hr.
- $\rightarrow$ So smog lives generally between 10am $\rightarrow$ 4pm.
- $\rightarrow$ ~~Forget~~ Still have NO_2 , organics, but by themselves they are not a problem.

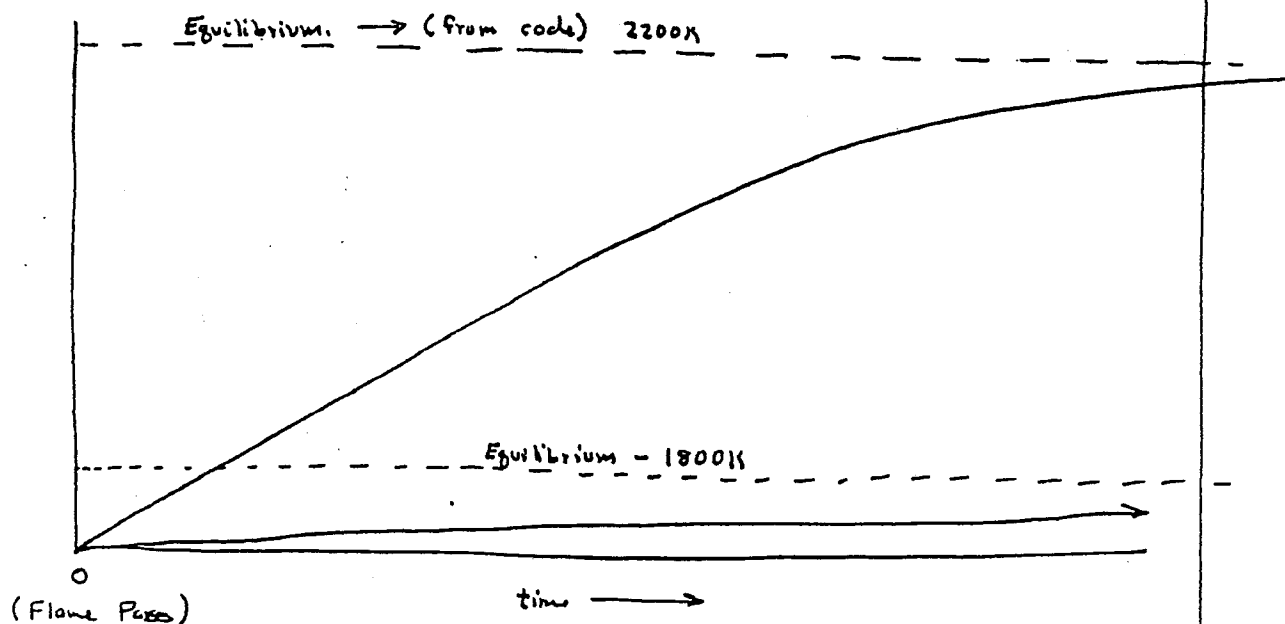
How do we make it? $\rightarrow$ All from fuel combustion. Two ways.

① Thermal NO: Make air hot enough and it will go $\rightarrow$ Doesn't directly depend on combustion:



Oct. 22

Defining characteristic: y_o depends on T
 rate at which 1st reaction goes depends on T . (why?)
 $\Rightarrow$ Look at auto cylinder.

 y_{NO} 

- Normally don't have enough time to reach equilibrium,
 $\Rightarrow$ Usually in linear growth regime

$T(K)$	Growth (ppm/s)
1800	74
2000	2200
2200	33,800

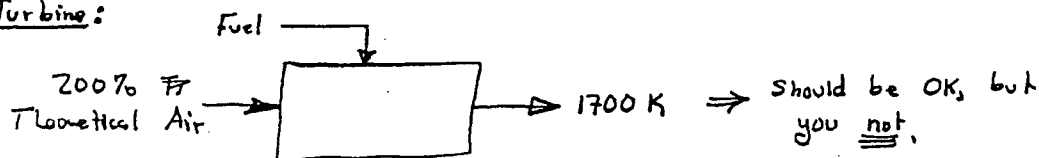
So how do you control?

- $\rightarrow$ Reduce peak T
- $\rightarrow$ Shorten time @ high- T .

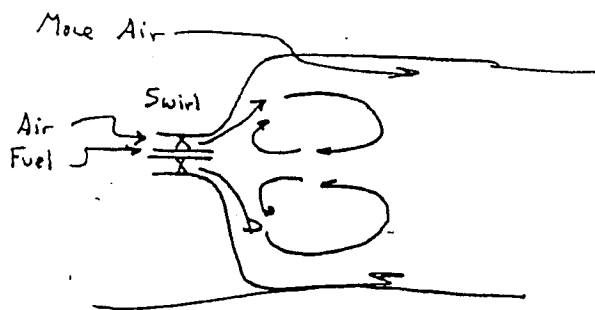
Auto is all thermal:

- $\rightarrow$ EGR- dilute
- $\rightarrow$ Retard spark timing ~~time~~
- $\rightarrow$ Reduce compression ratio.

Gas Turbine:

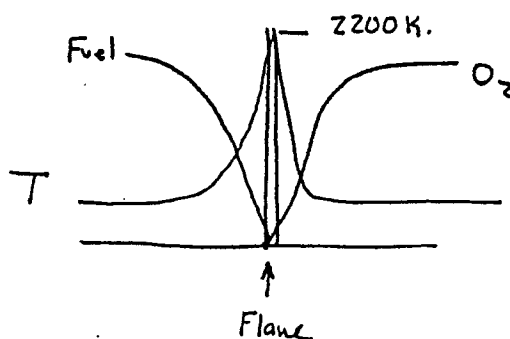
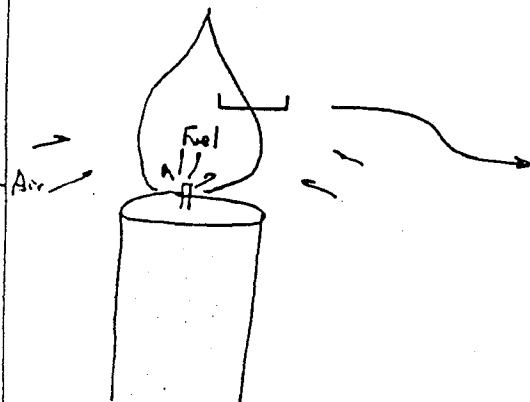


Classic gas turbine combustor:



- Main flame is closer to stoichiometric.
- Also, combustion is confined to planes where fuel and air meet.

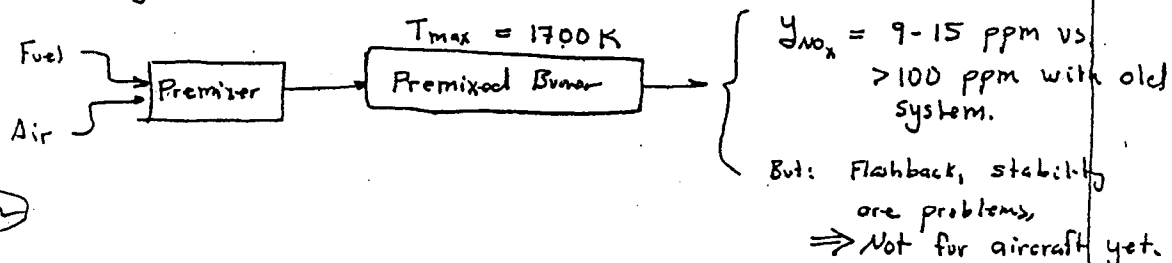
1700K



⇒ So flame occurs at stoichiometric rather than $\phi = 2$
(2200 vs. 1700K) ⇒ Lots of NO.

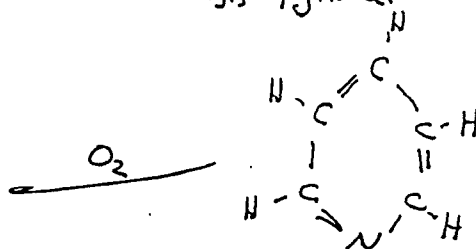
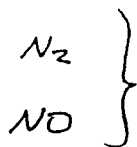
Modern systems:

Lean, premixed gas turbines:



② Fuel - Nitrogen:

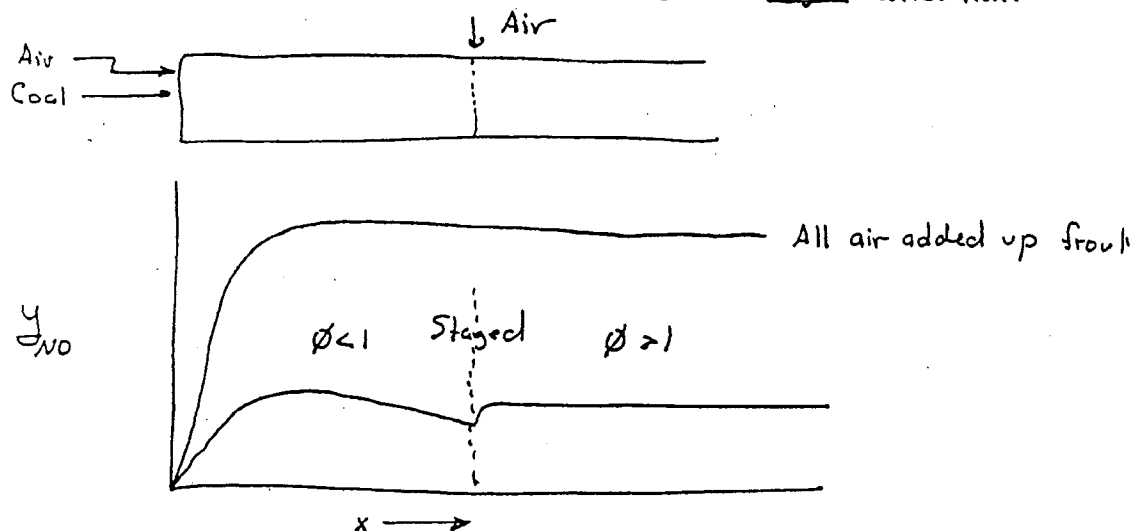
Cost ⇒ 1% N in organic part of fuel: e.g., pyridine.



Unlike thermal NO, don't need to break strong $\text{N}\equiv\text{N}$ bonds,
so don't need ~~high~~ high T.

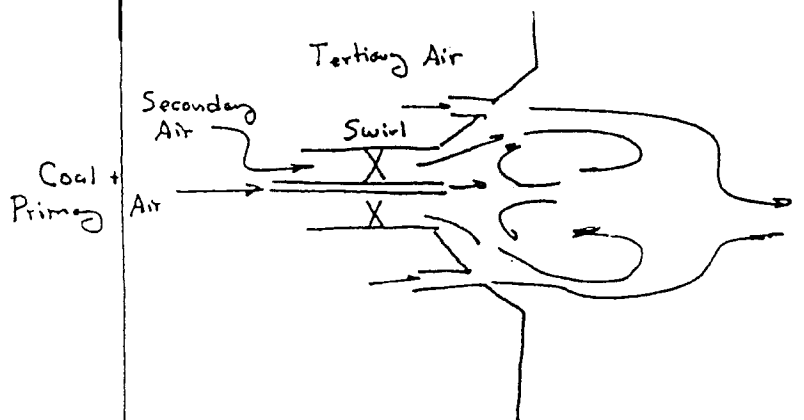
Observations: ① N_2 is favored over NO as amount of fuel-N goes up.
 ② N_2 " " " " at $\phi < 1$ (fuel-rich).

$\Rightarrow$ Can't do much with ①, but use ② in staged combustion.



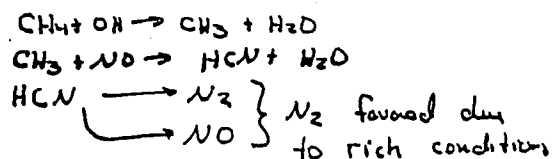
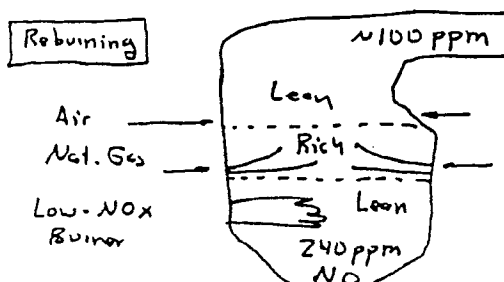
• Original idea exposes walls to $\phi < 1$ gas. This changes nature of ~~the~~ molten ash deposits and promotes boiler tube ~~to~~ corrosion.

• Same effect achieved via low- NO_x burner.



- Creates a rich inner core
Fuel N $\rightarrow N_2$
- Tertiary air finishes CO burnout.
- Easy retrofit: pull old burner off, put new one on.
- Must NO_x regs. can be met with this
- Performance:
600ppm $NO \rightarrow 240$ ppm.
- Problems:
 - $\rightarrow$ Longer flame
 - $\rightarrow$ Char harder to burn out.

Three other players:

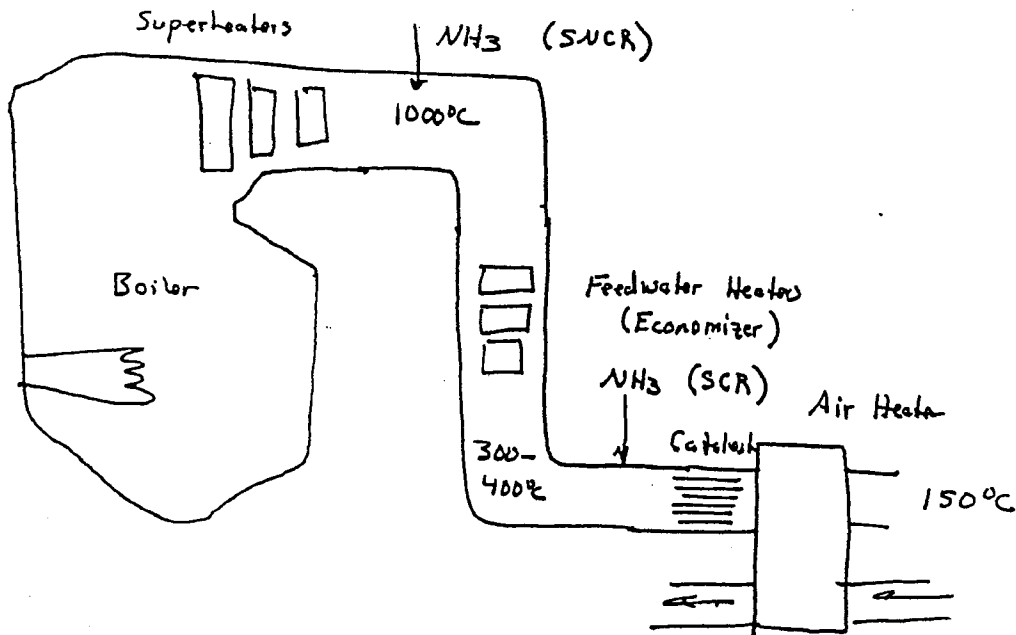


- Niche player $\rightarrow$ Moderate control
 - $\rightarrow$ Cheap
 - $\rightarrow$ Depends on clean NG .

Oct 25

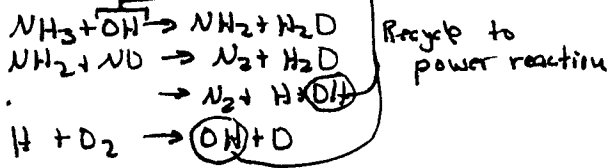
Selective Non-Catalytic Reduction SNCR

Selective Catalytic Reduction SCR

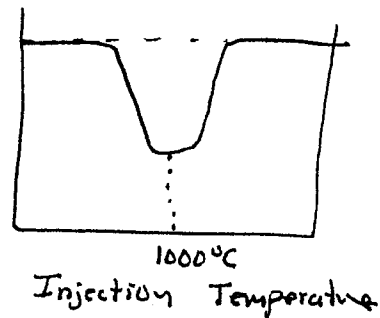


SNCR

- ~60% control
- Very cheap
- Challenges
 - Works over only a narrow T-range [Question: What problems might this cause?]
 - Pressurized NH_3
 - Slip and NH_4Cl plumes



$$\frac{y_{\text{NO}}}{y_{\text{NO},i}}$$



SCR

- V/Ti catalyst
- >90% reduction
- Expensive - Only apply when needed
- Reagen gas trouble good application.

Oct 26

Discuss
ExamRegulations Interesting.

• Impact is regional $\Rightarrow$ Key is controlling a sum of all sources to a given level
 $\rightarrow$ A single source doesn't matter.

• 600 MWe plant with 4% Illinois coal $\Rightarrow$ 148,000 tons SO_2 / yr.

• Government gives you ~~70,000~~ 62,000 "Allowances"

$\rightarrow$ 1 Allowance = licence to emit 1 ton SO_2 / yr. starting in 2002.

• Can buy and sell allowances. (current price $\approx$ \$150/allowance)
 \$150-300/ to 2004 | loss of banking
 Since to \$700

Market-Driven System.

• Build a scrubber $\Rightarrow$ 80% control $\Rightarrow$ Emit 30,000 tons/yr \$22.4E+6
 $\Rightarrow$ Sell 32,000 Allowances = \$4.8E+6

• Buy low-sulfur coal and blend to reach 62,000 tons/year.

• Buy 86,000 allowances on the open market = \$60.2E+6
 and do nothing.
~~\$12.9E+6~~

$\Rightarrow$ Economics: If your plant has only 5 yrs life left, buy allowances rather than building a scrubber.

$\Rightarrow$ Buy allowances for your friends.

Reactive Hydrocarbons

- CH_4 - non-reactive in troposphere.
- Others will react in smog cycle.
- Most sources are non-energy related (dry cleaning, painting, fast-food, charcoal lighter fluid).

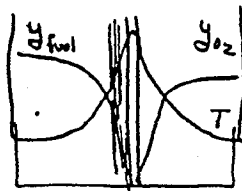
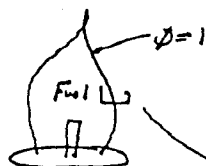
Auto is one example $\Rightarrow$ Cold walls } $\Rightarrow$ leaves unreacted fuel behind.
 $\Rightarrow$ Short time

Particulate Matter

- Two kinds

Soot:~~Fuel~~

Air

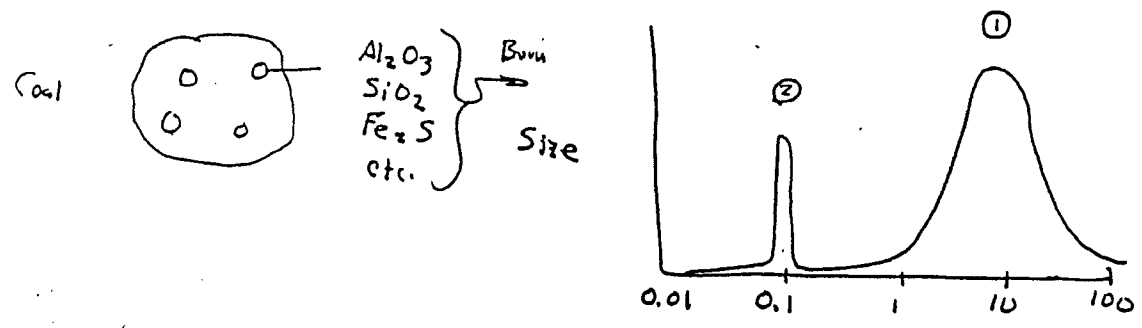


Hot, no $\text{O}_2 \rightarrow$ Fuel pyrolyzed to carbon particles.
 $\rightarrow$ Yellow is just black body radiation.
 $\rightarrow$ Usually those burn up.

Emissions: • Diesel
 • Bed combustion.

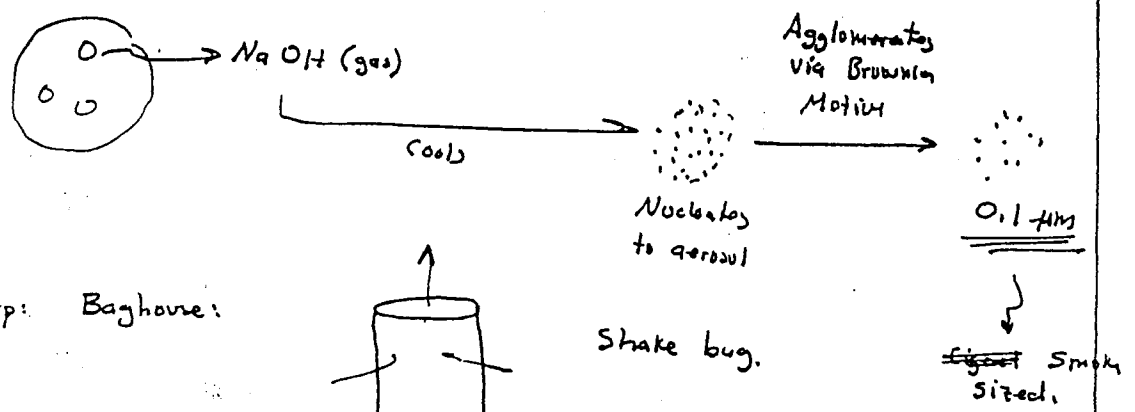
Oct. 29

Mineral based:

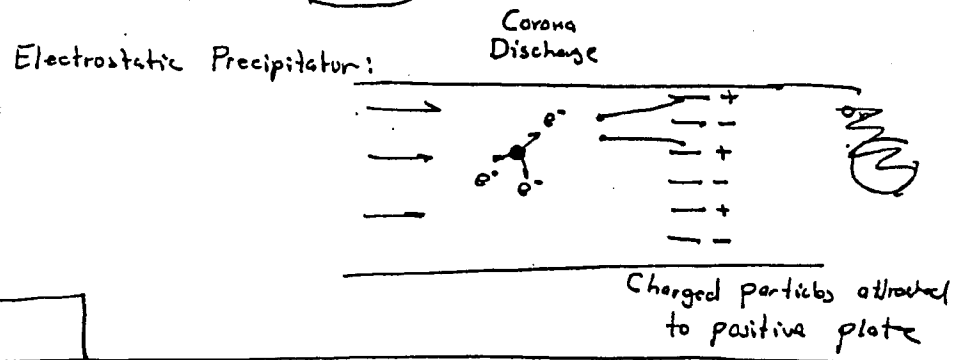
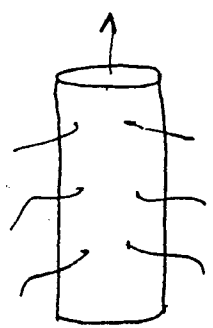


Mode ①: Coal burns out and minerals agglomerate.

Mode ②: Minerals vaporize



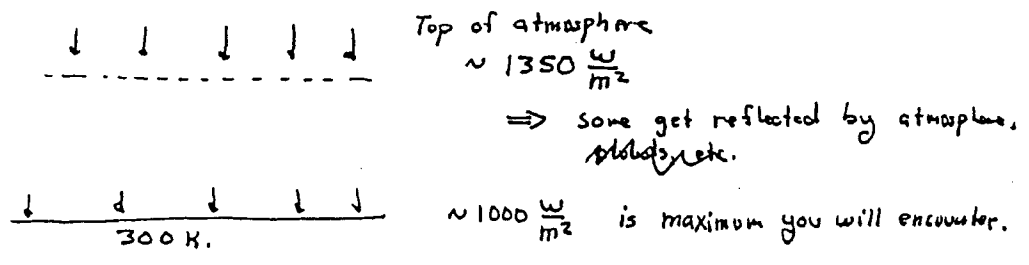
Cleanup: Baghouse:



Hg talk

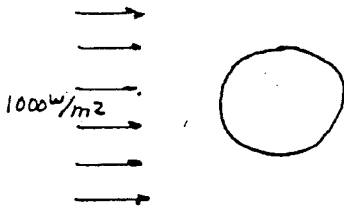
Greenhouse Gases $\Rightarrow$ What we know for sure.

Sun $\sim 6000 K$



Most incoming is $0.3 - 3 \mu\text{m}$
 Eyes see $0.4 - \text{Violet}$ to $0.7 - \text{Red}$ } Designed to see where the light is.
 $\Rightarrow$ Generally atmosphere is transparent to this stuff.

Simple earth model



Average over whole surface

$$\left. \begin{aligned} A_c &= \frac{\pi D^2}{4} \\ A_s &= \pi D^2 \end{aligned} \right\} \text{Average flux onto surface is } 250 \frac{\text{W}}{\text{m}^2}$$

At steady state, all this energy must be re-radiated back to space:

$$250 \frac{\text{W}}{\text{m}^2} = \underbrace{\sigma \epsilon}_{5.67 \times 10^{-8} \frac{\text{W}}{\text{m}^2 \cdot \text{K}^4}} [T_{\text{surf}}^4 - T_{\text{space}}^4] \Rightarrow T_{\text{surf}} = 258 \text{ K} \\ = -15^\circ \text{C} \\ = 5^\circ \text{F}$$

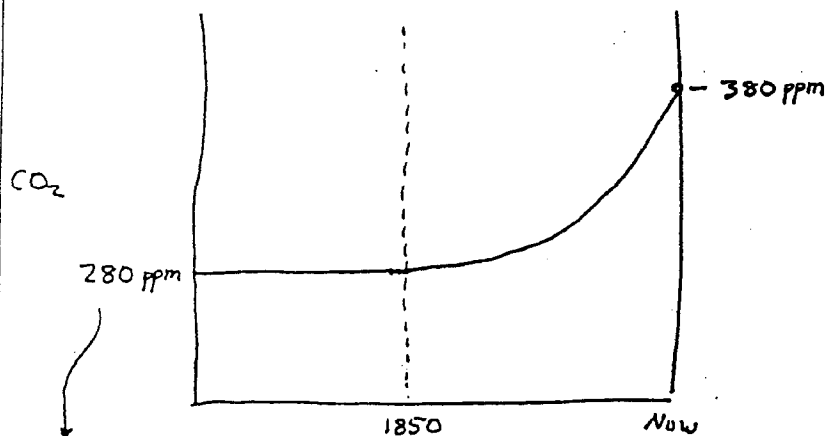
$\sim 4 \text{ K}$

$\Rightarrow$ So we need some help or we will get cold!

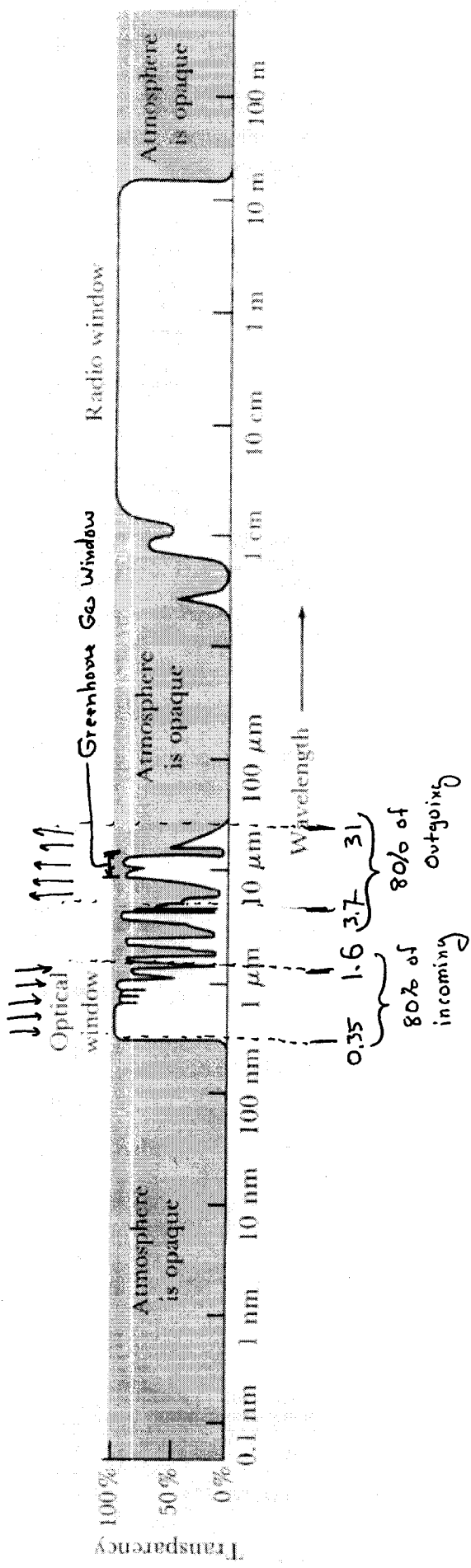
At 300 K , most reradiated energy is $3 - 31 \mu\text{m}$ (mid $\rightarrow$ deep IR)
 $\Rightarrow$ Atmosphere is opaque over most of this range (due to H_2O), but transparent window occurs at $7 - 13 \mu\text{m}$.
 $\Rightarrow$ Earth's steady-state temperature determined by balance between heat trapped lost in $7 - 13 \mu\text{m}$ vs. heat trapped outside this range.

But: $\left. \begin{array}{l} \text{CO}_2 \\ \text{N}_2\text{O} \\ \text{CH}_4 \\ \text{Freons} \end{array} \right\} \text{All absorb in } 7 - 13 \mu\text{m}, \text{ and these tend to plug the hole.}$

From atmospheric measurements and ice-core data, we know CO_2 has been increasing since ~ 1850 , coinciding with the large-scale use of fossil fuels.



Stable since end of last ice age.



- Tendency for warming leads to more evaporation from oceans.
[remember, $P_g \sim \exp(T)$]
⇒ Increased cloud cover ⇒ More reflection of solar radiation
- Models are very sensitive to this cloud-cover parameter.
i.e., a 5% change in average cloud cover swamps everything else.
⇒ This is why it seems folks can't make up their minds.
- Projected effect is more climate change than direct warming.
 - High ~~and~~ arctic gets warmer.
 - Some areas wetter, others dryer
 - Northwest ⇒ Wetter, warmer winters (less snow).
 - No icecap melting, but a couple of degree rise in ocean temps leads to thermal expansion ⇒ ~1m would be a problem.

What to do?

- Conserve: [Average tank of gas puts 300 lb CO₂ into atmosphere].
- Use power generation systems with higher η
- Use natural gas $C/H = 0.25$, For coal it's $C/H = 1$ ⇒ Half the CO₂ per KJ.
Wind, solar, biomass, tide, geothermal
- Renewables: Currently none are capable of replacing our dependence on fossil fuels
e.g. Biggest windfarm project in Northwest - Stebeline ⇒ 300 MW.
Total Washington capacity ⇒ 25,000 MW
⇒ Costs need to come down, technology needs to improve.
⇒ Value engineering.

Win

- Nuclear: No CO₂, can expand to cover the grid (France is ~80%).

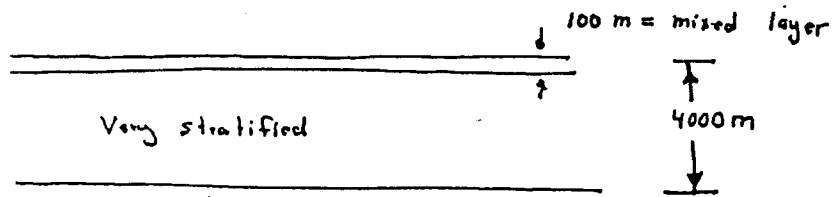
Oct. 31

Sequestration: Modify cycle to produce pure CO₂ as product (later)
→ Then what to do with it?

	10 ⁹ Tons	Uptake Rate / year
Look where it is now		
Atmosphere:	750	+ 6 produced.
Biosphere:	2000	- 2
Ocean Water:	39,000	- 2
Ocean Sediments	78,000,000	- 0.2

(Note: mass of ocean $\approx$ 8000x mass of air).

⇒ So there is plenty of room, and the limitation is on transport.



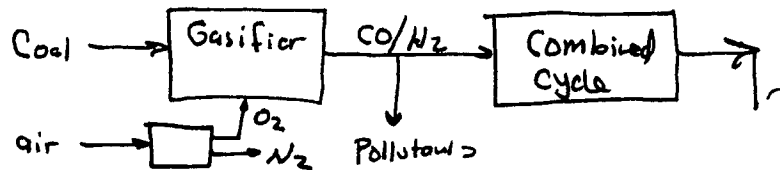
- ⇒ Top 100 m gets saturated, but mixing into lower layers is slow.
- ⇒ Mid or deep injection of liquid CO_2 .
 - Hydrates?
 - Oceanic inversion?
 - Ph problems?

Another approach → Deep coal mines or depleted oil wells.

⇒ All these require pure CO_2 to work well

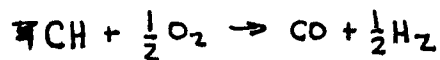
These lead towards Integrated Gasification Combined Cycle (IGCC)

- Domestic fuel (coal)
- Potential renewable (biomass)
- Higher efficiency than traditional Rankine
- Clean (?)
- CO₂ sequestration (?)



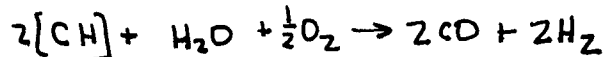
Many configurations - Will focus on one.

The gasifiers generally work by partial combustion. Treat coal as equimolar C/H

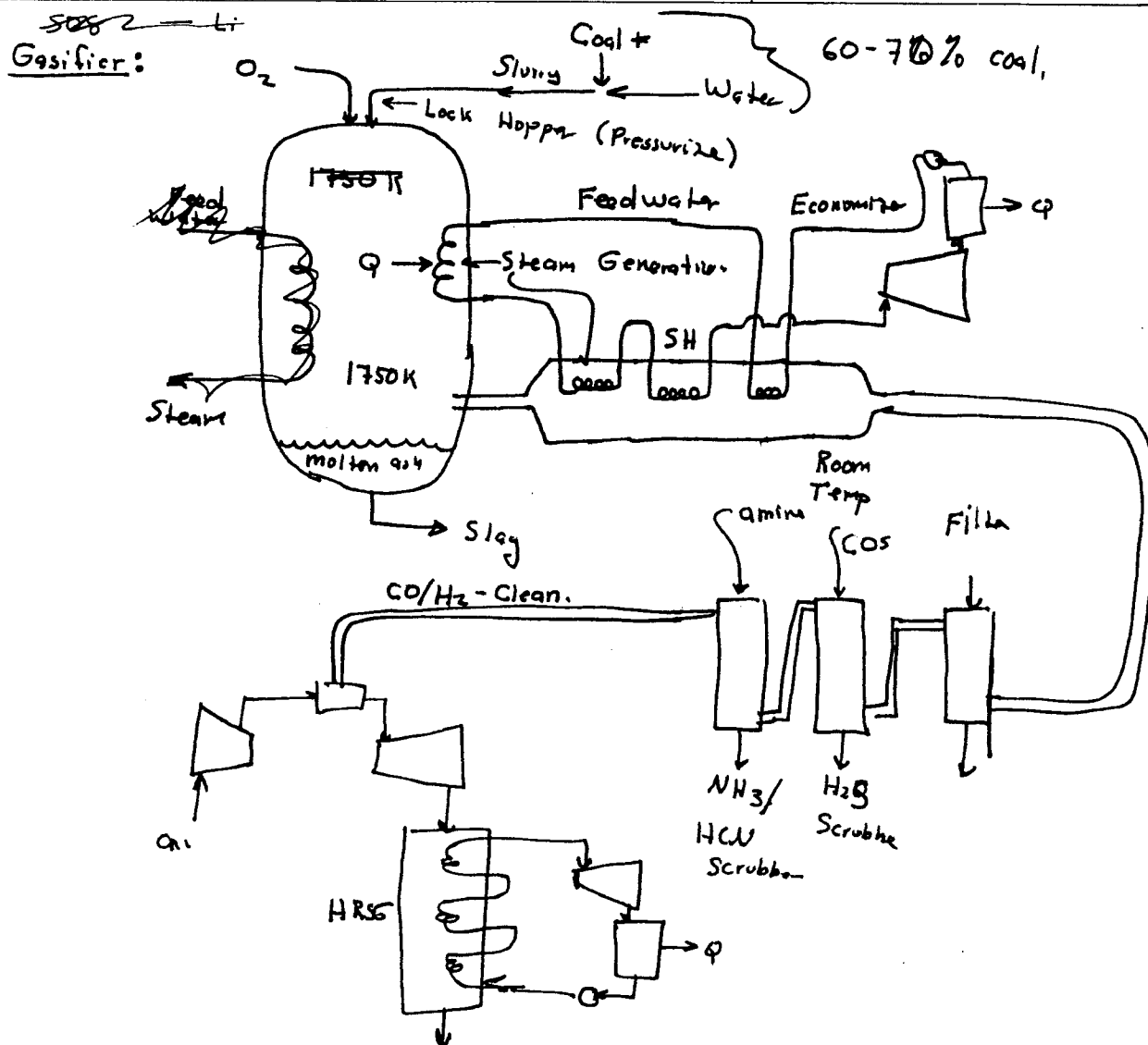


But (1) adiabatic flame T is too high,
(2) Prefer more H₂ than CO.

⇒ Add steam or water



Air separator → Cryogenic Distillation = 1.3 MJ/Kg O₂ produced.



Absolutely key point. Fuel gas flow rate is only $\sim 5\%$ of total plant gas flow, making all gasifier and cleanup equipment much smaller than otherwise.

Can integrate two steam cycles together.

Where is i ?

Options: air vs. O_2 blown gasification $\Rightarrow$ O_2 keeps fuel stream flow & cleanup cost down.

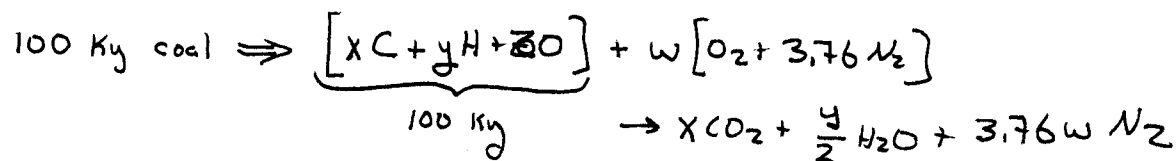
Pressure vs. atmospheric gasification $\Rightarrow$ Reduce size of fuel system, no compressor needed for fuel.

Gasifiers: Fluidized bed, entrained flow.
 $\Rightarrow$ minerals out bottom.

Cleanups: Ash, S needed for turbine blades. $\Rightarrow$ Goal is hot gas cleanup.
 Must presently use diffusion burners.
 H_2 - Fastest fuel } Mixing flow leads to confusion,
 CO - Slowest

- Advanced air separation (Hot membranes). $\Rightarrow$ Integrate into plant -
- Replace comb. with solid oxide fuel cell

Analysis:



Given LHV or HHV do calc.

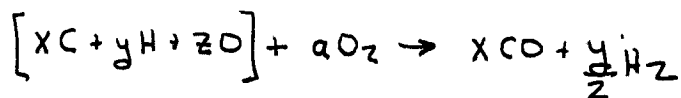
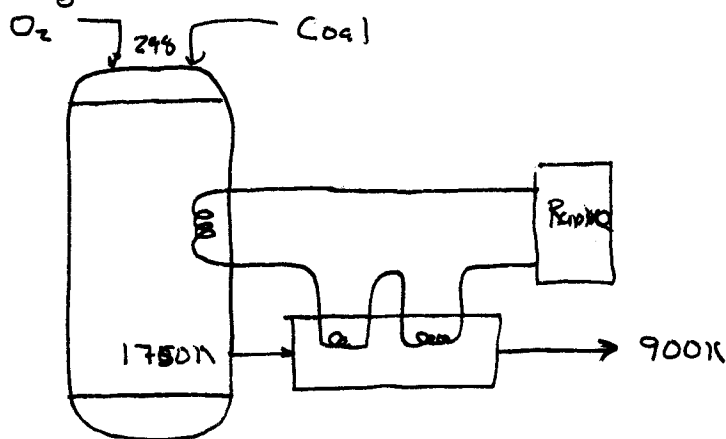
$$Q = H_P - H_R$$

$$Q = -LHV \text{ or } -HHV$$

$$H_P = xh_{f,CO_2} + \frac{y}{2} h_{f,H_2O}$$

$$H_R = h_{f,coal}$$

Now gasifier:



$$z + 2a = x \quad a = \frac{x-z}{2} \quad \checkmark$$

$$Q_{Rankine} = H_P - H_R$$

Species	h_f°	$h - h_{298}$	
Coal	$h_{f,coal}$	0	] = H_R
O_2	0	0	
CO	-110,530	$h_{900} - h_{298}$	
H_2	0	$h_{900} - h_{298}$	] = H_P

$\Rightarrow$ OFC to gas turbine, all else is the same -

Where is the i?

• Reaction in gasifier

• large ΔT for g in gasifier

Also, cold gas cleanup means must use more fuel to reach target T @ turbine inlet.

$\Rightarrow$ Big goal is hot gas cleanup.

$\Rightarrow$ These hits put you @ $\sim 45\%$ efficiency.

Economics

	NGCC	IGCC	Modern Rankine
Capital (\$/kW)	500	1050	1100
$\uparrow$	60	45	37
Uncertainty	NG costs	low	future env. regs.

Coal costs invariant. Also, integrated cleanup leads to very low emissions.

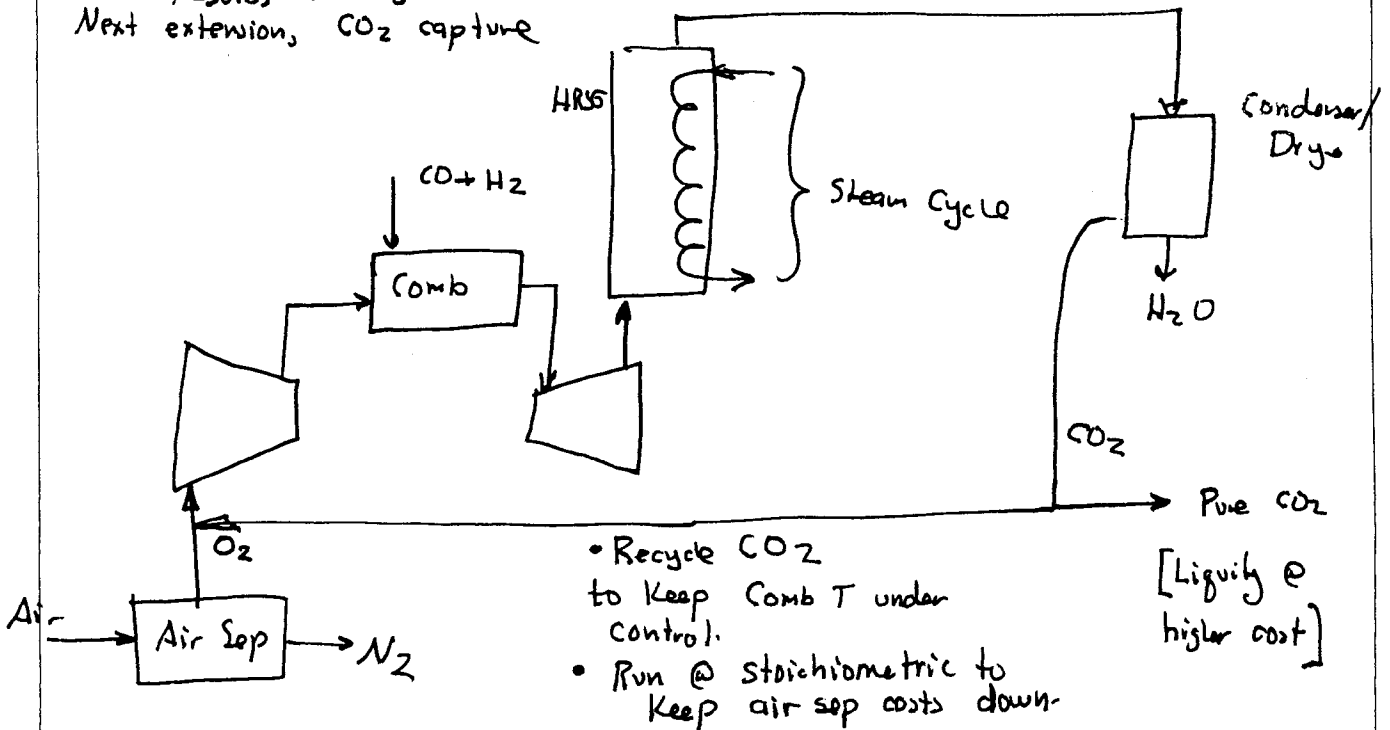
Lets see how it works: 600 MWe, 20 yr life, 6% interest

	IGCC	NGCC
Capital	\$630 E+6	\$300 E+6
Annual Cost Cap.	\$54.9 E+6	\$26.2 E+6
Fuel:	\$50.0 E+6	\$78.7 E+6
Total Annual	\$104.9 E+6	104.9 E+6

\$78.7 E+6	\$	0.6 KJ _e	KJ _{th}	10 ⁶ BTU	yr
yr	600,000 KJ _e	KJ _{th}	0.9478 BTU	[10 ⁶ BTU]	31.5 E+6

= \$2.64 \$/10⁶ BTU
@ break even.

Absorb, or oxyfuel -
Next extension, CO₂ capture



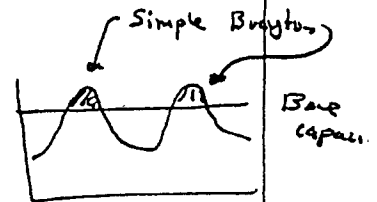
Nov 2

So: Rankine: Large present capacity, but little construction

- Low η
- Cheap fuel
- Environmental cleanup expensive due to huge gas flows.

Simple Brayton:

- Low η
- Expensive fuel
- Low capital cost.
- Used to cover peak demands



Combined Cycle Gas Turbines: volatile

- Expensive fuel, high η
- No cleanup needed
- Moderate capital
- ~~Most~~

IGCC: ↑

- Cheap, stable fuel
- Moderate η
- Cleanup cheap (for coal) since work only on ~~an~~ fuel stream.
- Possible choice if gas gets pinched. → Still needs tech development

Nuclear:

- ~ 20% of electricity
- No CO₂

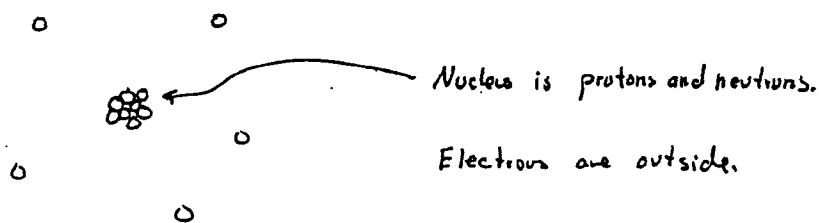
Some now feeling this is the lesser evil.

~~Nuclear Power~~

Nuclear Power

- Atomic reactions: Mass and energy balances
- Radioactive decay
- Fission
- Reactor design fundamentals
- Reactor types
- Accidents.

The atom:



Protons have "+" charge } $\sim 1.68 \times 10^{-27} \text{ Kg}$
 Neutrons have no charge }

Electrons have "-" charge $\sim 9.12 \times 10^{-31} \text{ Kg}$
 $\sim 1800 \times$ difference.

$\Rightarrow$ Most mass is in nucleus.

$\Rightarrow$ Element determined by # of protons: $H=1$
 $He=2$

$\Rightarrow$ Isotope by # of neutrons

	P	N
Hydrogen	1	0
Deuterium	1	1
Tritium	1	2

Convention: $\begin{matrix} 3 \\ \curvearrowright \\ 1 \end{matrix} H$ Protons + Neutrons = Nucleons = Total nuclear particle count.
 $\begin{matrix} 12 \\ \curvearrowright \\ 6 \end{matrix} C$ Carbon-12 $\Rightarrow \begin{matrix} 12 \\ 6 \end{matrix} C$

To make mass numbers manageable, atomic masses are given in AMU
 $=$ Atomic mass unit $1 \text{ AMU} \cong$ mass of proton or ~~electron~~ neutron.

Formal definition: 1 atom of Carbon-12 $\equiv$ ~~12 AMU~~ 12 AMU
 (6 protons, 6 electrons, 6 neutrons).

Get conversion between AMU and kg $\Rightarrow$

$$\frac{12 \text{ AMU}}{\text{atom C}} \mid \frac{6.023 \times 10^{26} \text{ atoms C}}{\text{K mole C}} \mid \frac{\text{K mole}}{12 \text{ kg C}} = \boxed{6.023 \times 10^{26} \frac{\text{AMU}}{\text{kg}}}$$

From isotope table (link will be on website)

$$\begin{array}{lcl} {}^1_1\text{H} & (\text{proton + electron}) & \text{weighs } [1.007825 \text{ AMU}] \\ {}^1_0\text{n} & (\text{neutron}) & \text{weighs } [1.008665 \text{ AMU}] \end{array}$$

Lets make ${}^{12}_6\text{C}$ $\Sigma = 12.09894 \text{ AMU}$

Why doesn't this add to 12.00? Missing mass from our hypothetical reaction was converted to energy.

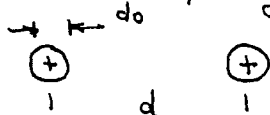
Get via:

$$E = mc^2 = \frac{0.09894 \text{ AMU} \times \text{Kg}}{6.023 \times 10^{26} \text{ AMU}} \left[\frac{3.0 \times 10^8 \text{ m}}{\text{s}} \right]^2 = 1.48 \times 10^{-11} \text{ J}$$

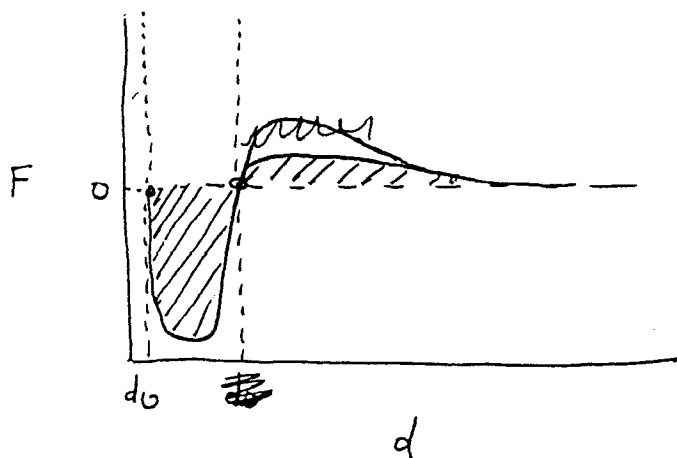
So our hypothetical nuclear reaction is:



Why? Think about pushing two protons together

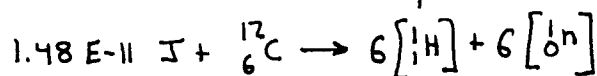


Lets push those together.



1. As we bring them together, they repulse due to coulomb forces.
2. At very close distances, they attract due to the "strong" force.
3. Pauli exclusion principle prevents occupation of same space.

Easier to think about reverse process: Start together and pull apart $W = \int_{d_0}^{\infty} F dx$



Input energy $\Rightarrow$ Extra mass.

"unbinding" energy?

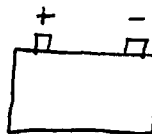
Binding Energy = Energy ~~needed~~ needed to unbind nucleus.

$\Rightarrow$ nucleus is lower energy than components [like $\text{O} + \text{O}$ vs. O_2]
 $\Rightarrow$ Larger the binding energy, the more stable the nucleus.

Just like we use AMU = mass, Electron volt = energy.

$$1 \text{ Volt} = \frac{1 \text{ Joule}}{\text{Coulomb}}$$

$$[1 \text{ Coul} = 6.25 \times 10^{18} \text{ electrons}]$$



12 volts means it takes 12 J to move 1 coulomb from + to -.

Electron volt $\equiv$ energy needed to move 1 electron across 1 volt.

$$\frac{1 \text{ electron}}{1 \text{ Coul}} \times \frac{1 \text{ J}}{6.25 \times 10^{18} \text{ electrons}} = 1.60 \times 10^{-19} \text{ J/eV}$$

$$= \boxed{1.60 \times 10^{-13} \text{ J/MEV}}$$

(MEV = 10^6 eV)

So we have two kinds of mass units: kg, AMU
" energy " J, MEV

Conversions: $6.023 \times 10^{26} \frac{\text{AMU}}{\text{kg}} \quad 1.60 \times 10^{-13} \frac{\text{J}}{\text{MEV}}$

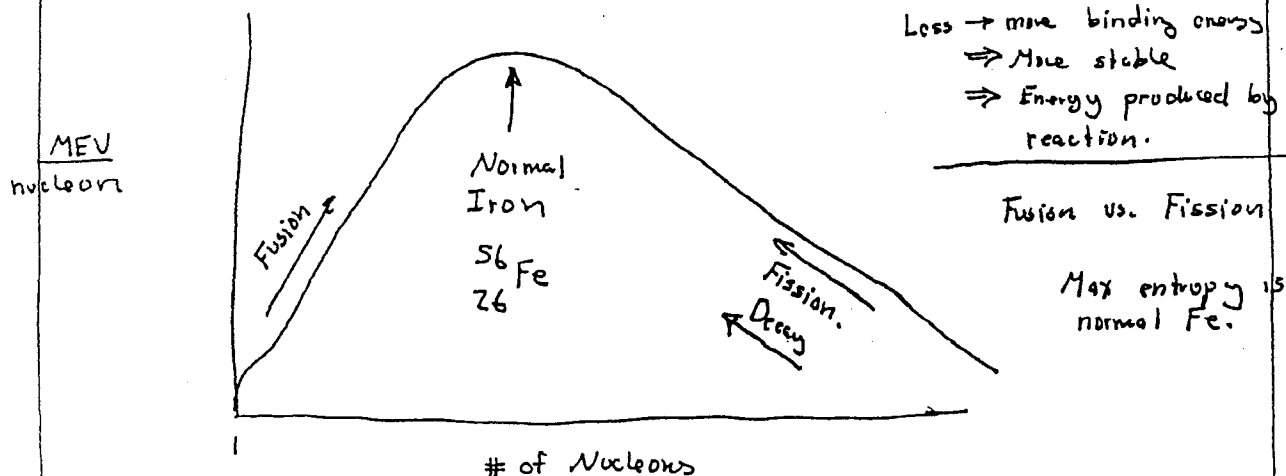
mass $\leftrightarrow$ energy

$$E = mc^2 = \frac{1 \text{ kg} \left[\frac{3.0 \times 10^8 \text{ m}}{\text{s}} \right]^2}{1} = 8.99 \times 10^{16} \text{ J/kg}$$

$$1 \text{ AMU} = 1.66 \times 10^{-27} \text{ kg} = 1.49 \times 10^{-10} \text{ J} = 934 \text{ MEV}$$

	J	MEV
kg $\leftrightarrow$	$8.99 \times 10^{16} \text{ J/kg}$	$5.63 \times 10^{29} \text{ MEV/kg}$
AMU	$1.49 \times 10^{-10} \text{ J/AMU}$	934 MEV/AMU

Now plot binding energy/nucleon (prot + neut) vs. # of nucleons
 $\Rightarrow$ Average binding $\frac{E}{A}$ / nucleon



Nov. 5

Three types of nuclear reactions

Fusion: ${}^2_1\text{H} + {}^2_1\text{H} \rightarrow {}^4_2\text{He}$ } ^{"+"}
 • Pushing two charged nuclei together
 • Requires high KE $\Rightarrow$ Very high temperature.

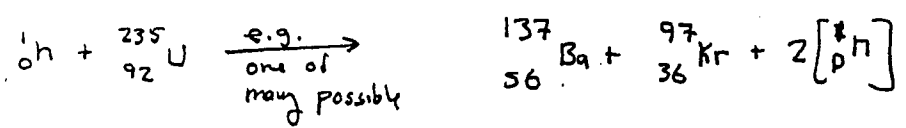
Decay: ${}^{238}_{92}\text{U} \xrightarrow{4.5 \times 10^9 \text{ yr}} {}^4_2\text{He} + {}^{234}_{90}\text{Th}$
 (1) α -decay: $\Rightarrow \alpha$ penetration weak ~~unimportant~~

(2) β -decay: ${}^{197}_{78}\text{Pt} \xrightarrow{18 \text{ hr}} {}^{197}_{79}\text{Au} + \beta^-$ } ${}^1_0\text{n} \rightarrow \text{Proton} + \text{electron}.$
 $\Rightarrow$ ~~Proton~~ stays, while electron leaves with high KE $\Rightarrow$ Can do a lot of damage

(3) Positron decay } Not important for power.
 (4) K-capture }

$\Rightarrow$ In decay, material just sits there and gives off heat
 $\Rightarrow$ Recent story from Russia about Sr-90 batteries.

Fission: Neutron hits fuel and breaks nucleus (makes 2 or 3 neutrons).

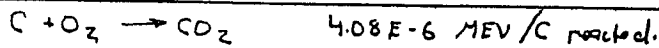


- Released ${}^1_0\text{n}$ can do more reactions $\Rightarrow$ Chain mechanism
- Ba, Kr are radioactive, will decay giving more energy.
- Only ${}^{235}_{92}\text{U}$, ${}^{233}_{92}\text{U}$, ${}^{239}_{94}\text{Pu}$ } are really capable of doing this.
- Huge family of products are made

$\Rightarrow$ Average fission + average subsequent decay $\cong$ 200 MEV/fission.

R $\left[\begin{array}{l} {}^1_0\text{n} - 1.008665 \text{ AMU} \\ {}^{235}_{92}\text{U} - 235.0439 \end{array} \right] R = 236.052565$
 P $\left[\begin{array}{l} {}^{137}_{56}\text{Ba} - 136.9058 \\ {}^{97}_{36}\text{Kr} - 96.9262 \\ 2({}^1_0\text{n}) = 2.01733 \end{array} \right] P = 235.84933$
 $\Delta m = 0.2032 \text{ AMU}$

Energy Release: $\frac{0.2032 \text{ AMU} \times 934 \text{ MEV/AMU}}{\text{AMU}} = 189.8 \text{ MEV/fission (+ decay)}.$

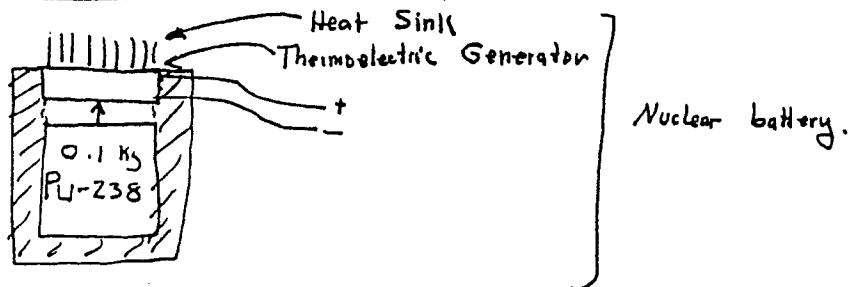


Note that a 600 MW coal plant uses $4800 \frac{\text{tons C}}{\text{day}}$.

releasing: $144. E+6$ MJ/day. $\Rightarrow$ Relative mass loss is 1.6 g !
($3.3E-10$ factor)

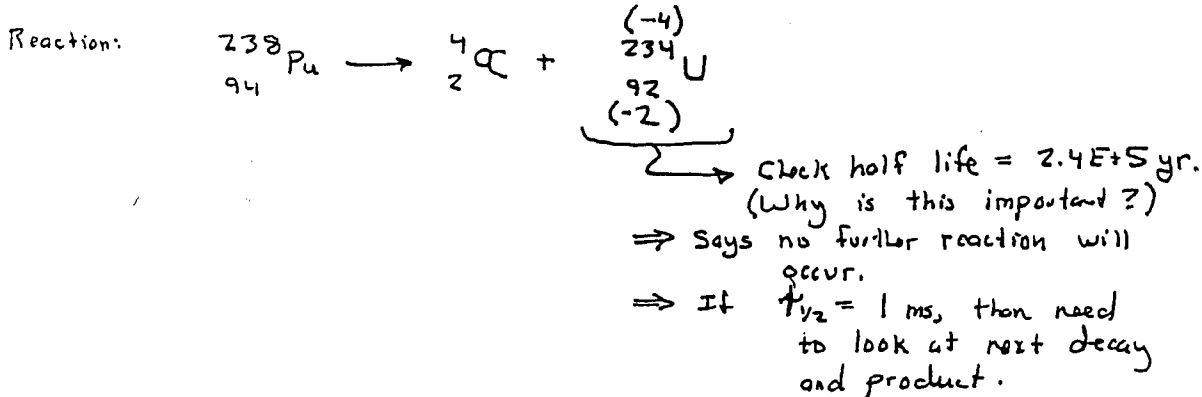
Fuel	Energy (MJ/kg)
Coal	30
$^{235}_{92}\text{U}$	$82E+6$
^3_1H	$574E+6$

Decay:



Look up website: $^{238}_{94}\text{Pu}$ $\left\{ \begin{array}{l} \text{mass} = 238.04955 \text{ AMU} \\ t_{1/2} = 87.74 \text{ yr} \\ \propto \text{decay.} \end{array} \right.$

This is all the info you need to get power output!



Energy release:	$^{238}_{94}\text{Pu}$	238.04955	$\left. \begin{array}{l} \text{R} \\ \text{P} \end{array} \right\} \Delta m = 0.0060032 \text{ AMU}$
	$^4_2\alpha$	4.0026	
	$^{234}_{92}\text{U}$	234.0409468	

Energy/decay = $\frac{0.0060032 \text{ AMU}}{\text{decay}} \left| \frac{934 \text{ MEV}}{\text{AMU}} \right. = 5.607 \frac{\text{MEV}}{\text{decay}} \Rightarrow \boxed{2.0E+6 \frac{\text{MJ}}{\text{kg}}}$

Compare to above

Now we need to use the half life to get the rate of energy production:

Rate of reaction $\sim$ number of atoms of Pu-238 present

"-" because atoms $= -\lambda N$ $\left\{ \begin{array}{l} \text{Atoms} \\ \text{constant (to be)} \end{array} \right.$

The way we get power is $= \left[\frac{\text{decays}}{s} \right] \left[\frac{\text{energy}}{\text{decay}} \right]$

decay rate $\left[\frac{\text{atoms decaying}}{s} \right] \sim \text{size of sample} \left[\begin{array}{l} \text{double size, double} \\ \text{decays} \end{array} \right]$

$$\frac{dN}{dt} = -\lambda N$$

$N = \text{atoms in sample}$

$\lambda = \text{proportionality constant to be determined.}$

$$\frac{dN}{N} = -\lambda dt, \quad \int_{N_i}^N \frac{dN}{N} = - \int_0^t \lambda dt$$

$$\ln \left[\frac{N}{N_i} \right] = -\lambda t \quad \text{or} \quad \frac{N}{N_i} = \exp[-\lambda t]$$

$\Rightarrow$ Exponential decay



λ has units s^{-1} , so let $\lambda = \frac{1}{\tau^*}$ where $\tau^* = \text{characteristic decay time} (\neq \tau_{1/2})$.

Now get τ^* from $\tau_{1/2}$

$$\frac{N}{N_i} = \exp \left[-\frac{t}{\tau^*} \right] \Rightarrow 0.5 = \exp \left[-\frac{\tau_{1/2}}{\tau^*} \right] \Rightarrow \tau^* = -\frac{\tau_{1/2}}{\ln(0.5)}$$

$$\text{Power} = \left[\frac{dN}{dt} \right] \left[5.607 \frac{\text{MEV}}{\text{decay}} \right]$$

$$\Rightarrow \tau_{1/2} = 87.74 \text{ yr}$$

$$\Rightarrow \tau^* = 126.58 \text{ yr}$$

$$N = N_i \exp \left[-\frac{t}{\tau^*} \right] \Rightarrow \frac{dN}{dt} = -\frac{N_i}{\tau^*} \exp \left[-\frac{t}{\tau^*} \right]$$

$$\text{Power} = N_i = \frac{0.1 \text{ kg}}{238 \text{ kg}} \left| \frac{\text{Kmol}}{\text{Kmol}} \right| \frac{6.023 \times 10^{26} \text{ atoms}}{\text{Kmol}} = 2.53 \times 10^{23} \text{ atoms}$$

$$\text{Power} = \frac{5.607 \text{ MEV}}{\text{atom}} \left| \frac{2.53 \times 10^{23} \text{ atoms}}{126.58 \text{ yr}} \right| \frac{\text{yr}}{31.5 \times 10^6 \text{ s}} \exp \left[-\frac{0}{126.58 \text{ yr}} \right]$$

$$= 3.56 \times 10^{14} \text{ MEV/s.}$$

$$\frac{3.56 \times 10^{14} \text{ MEV}}{s} \left| \frac{1.60 \times 10^{-13} \text{ J}}{\text{MEV}} \right| = 56.9 \text{ W @ } t=0$$

over time

$$\text{Power} = [56.9 \text{ W}] \exp \left[-\frac{t}{126.58 \text{ yr}} \right]$$

in 88 yr,

Power will be half.

Things to consider:

- ① If you want minimum power at end of life, must overdesign at start:

150 W @ 10 years:

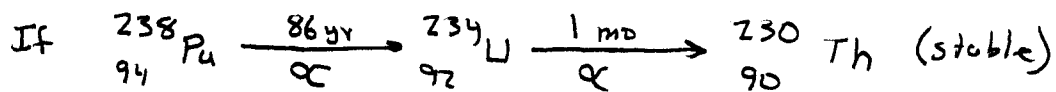
$$\text{Power} = \left[\frac{\text{MEV}}{\text{decay}} \right] \left[\frac{N_i}{\tau} \right] \exp \left[-\frac{t}{\tau} \right]$$

$$150 \text{ W} = \frac{5.607 \text{ MEV}}{\text{atom}} \left| \frac{N_i}{126.58 \text{ yr}} \right| \frac{\text{yr}}{31.536 \text{ s}} \left| \frac{1.60 \text{ E-13 J}}{\text{MEV}} \right| \exp \left[-\frac{10}{126.58} \right]$$

$$\Rightarrow N_i = \frac{7.21 \text{ E+23 atoms}}{6.023 \text{ E+26 atoms}} \left| \frac{\text{kmol}}{\text{kmol}} \right| \frac{238 \text{ kg}}{238 \text{ kg}} = \underline{\underline{0.285 \text{ kg}}}$$

Nov 7

- ② If product is unstable, with much shorter half-life, assume it immediately goes to next product.



$$\text{then get } \frac{\text{MEV}}{\text{decay}} \text{ from } = m_{\text{Pu}} - m_{\text{Th}} - 2m_{\alpha}$$

- ③ α will create He, which must be vented.

Fission: $^1_0n + \text{Fuel} \rightarrow \text{Prod 1} + \text{Prod 2} + [2 \text{ or } 3] ^1_0n$

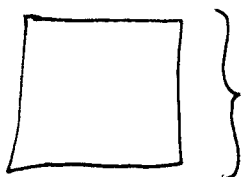
3 fuels: $^{235}_{92}\text{U}$, $^{239}_{94}\text{Pu}$, $^{233}_{92}\text{U}$

$\rightarrow$ Only natural isotope.

Natural uranium:

U-238	99.274%
U-235	0.720
U-234	0.006

$\frac{1}{2} \text{ yr}$
 $5.0 \text{ E} + 9$
 $7.0 \text{ E} + 8$
 $2.4 \text{ E} + 5$ } Original complement.



Reactor is in balance as long as ^1_0n production = ^1_0n consumption.

Production
 $\Rightarrow$ Fission

Consumption
 $\Rightarrow$ Fission
 $\Rightarrow$ Capture by U-238 et. al.
 $\Rightarrow$ loss out reactor.

$\Rightarrow$ Natural uranium has too little U-235, too much 238 to balance, except in heavy water reactor (CANDU).

$\Rightarrow$ Need to pull U-235 out - enrich. 3-5% for reactor, >20% for weapons

$\Rightarrow$ Chemical props the same, so chemical separation won't work.

$\Rightarrow$ Need to rely on mass difference.

~~$\Rightarrow$ lighter U~~

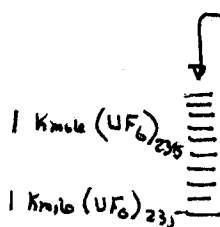
Proliferation a problem, so will pay attention to weapons.

Convert raw U $\rightarrow \text{UF}_6$ (a gas).

MW UF_6 $\frac{\text{U-238}}{352}$ $\frac{\text{U-235}}{349}$ } ratio = 1.0086

$$KE_{238} = KE_{235} \quad m_{238} V_{238}^2 = m_{235} V_{235}^2$$

$$1.0086 = \left(\frac{V_{235}}{V_{238}} \right)^2 \Rightarrow \frac{V_{235}}{V_{238}} = 1.0043$$

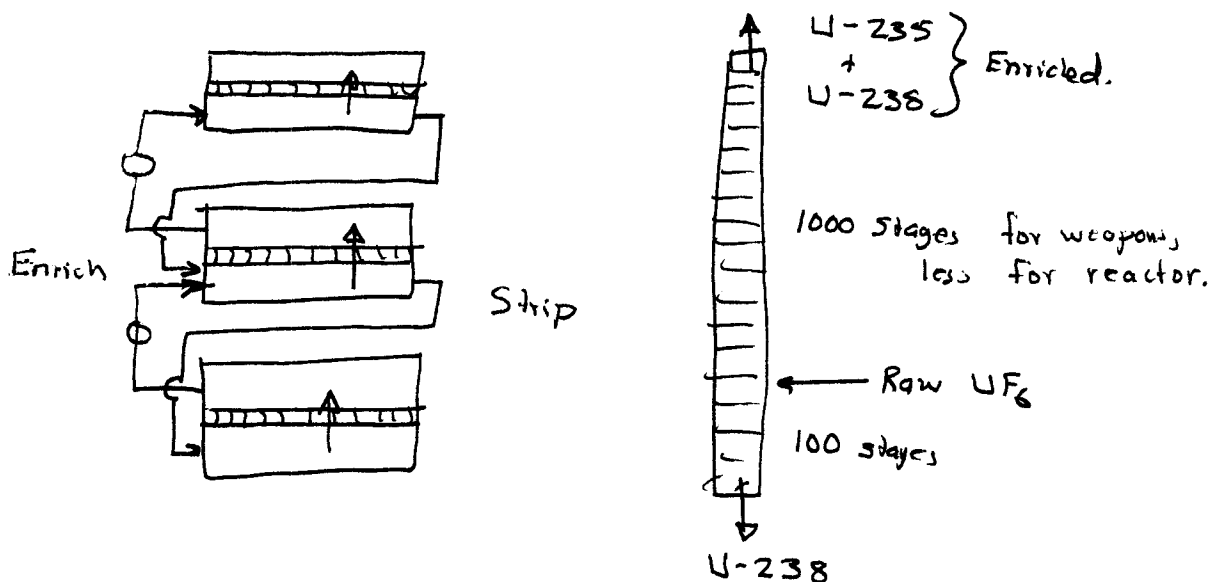


Because of higher speed

$1.0043 \times (\text{UF}_6)_{235}$ will cross barrier relative to $(\text{UF}_6)_{238}$

$\Rightarrow$ Ideal single stage enrichment.





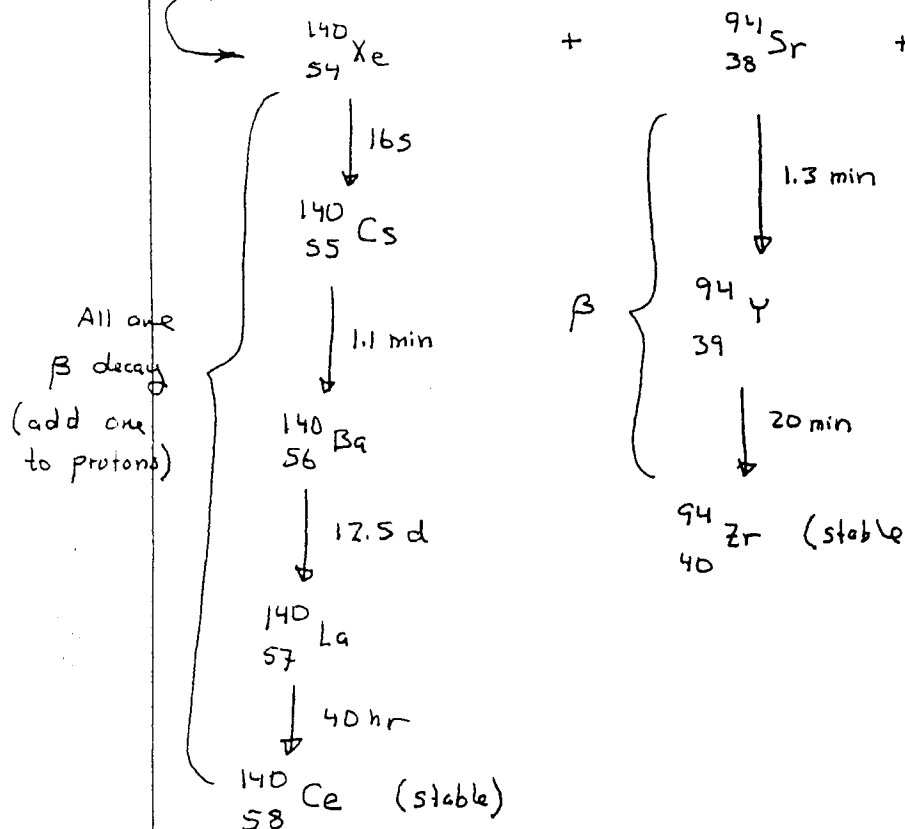
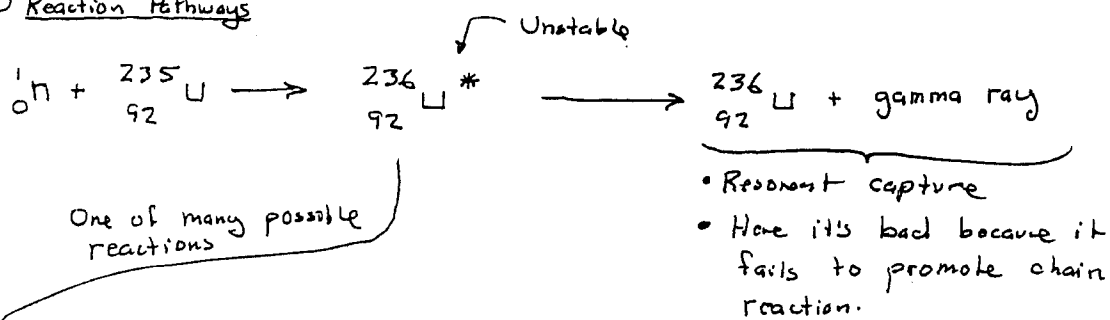
React UF_6 to UO_2 and put in pellets
(MP 2880°C)

Depleted U-238 $\rho = 19 \text{ g/cc}$ vs. $\text{Pb} = 11$.

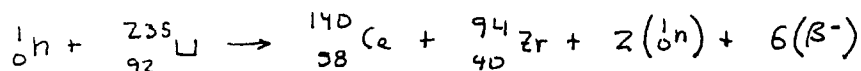
Will Cover the following topics.

- ① Reaction pathways
- ② Neutron speed control
- ③ Cross-sections: Choice of materials.
- ④ Budget for 1000 neutrons
- ⑤ Reactor kinetics/control
- ⑥ Common reactor designs
- ⑦ Accidents

① Reaction Pathways



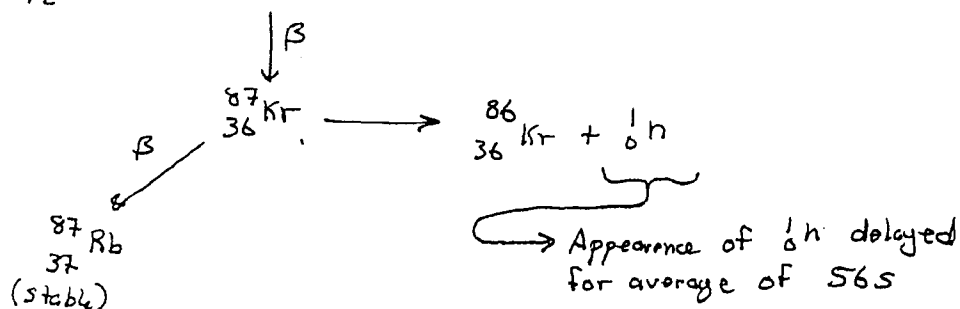
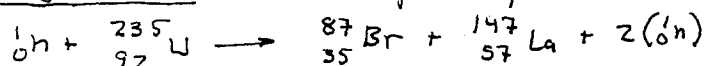
So overall we have:



Get $m_{\text{R}} - m_{\text{P}} = 0.2205 \text{ AMU} = 205 \frac{\text{MEV}}{\text{fission}}$

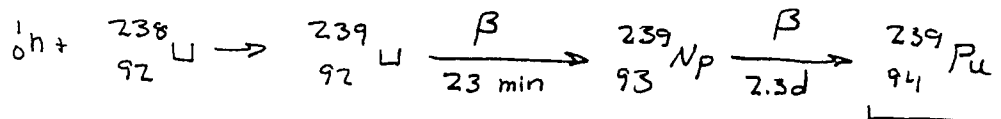
$\Rightarrow$ Neutrons produced are very high energy (fast speed $\rightarrow$ fast neutrons).

Delayed neutron - Another important path:



- ⇒ Time constant for main reaction is very short
 - ⇒ Cannot be mechanically controlled
- ⇒ Delayed neutrons give average ~~the~~ response time that is controllable.
- ⇒ Also, off really isn't off (delayed neutrons + decay).

Breeding: Fuel a mix of U-235 + U-238



⇒ Made a fissionable fuel out of useless U-238?

Three applications:

- ① Normal reactor: New Pu-239 extends fuel life by adding new fuel as U-235 is depleted.
- ② Can separate out Pu-239 for bombs (Hanford)
- ③ Can design breeder reactor that makes more Pu-239 than U-235 is lost ⇒ Makes more fuel than it consumes
⇒ Makes U-238 an energy resource.

Key points:

- Chain reaction promoted by more ${}^1_0n$ in products than reactants
- Immediate products undergo decay → more energy
- Delayed ${}^1_0n$ important for control
- U-238 capture of ${}^1_0n$ → new fuel (${}^{239}_{94}\text{Pu}$).

Nov. 8

② Neutron Speeds:



- No charges, so no coulomb repulsion to overcome
 - Will a fast or slow ${}^1_0n$ be more likely to be captured?
- ⇒ Slow is much more reactive.
- ⇒ But ${}^1_0n$ from reaction are fast.

⇒ Need two kinds of ${}^1_0n$ interaction in core.

- ① Moderator - slow down ${}^1_0n$
- ② Control - Absorb ${}^1_0n$ to control power density.

${}^1_0n$ behave like a monatomic ideal gas, so we can get speed from T.

$$\bar{u} = \bar{C}_v T, \text{ but for monatomic ideal gas } \bar{C}_v = \frac{3}{2} \bar{R}$$

$$\Rightarrow \bar{u} = \frac{3}{2} \bar{R} T$$

Only place ${}^1_0n$ can place energy is in translation.

$$\bar{u} = \frac{1}{2} m v^2 = \frac{3}{2} \bar{R} T \quad \text{mass of 1 kmole } {}^1_0n$$

$$\Rightarrow v = \left[\frac{3RT}{m} \right]^{1/2} = \left[\frac{3 \cdot 8.314 \text{ kJ} \cdot \text{K}^{-1} \cdot 300 \text{ K}}{1 \text{ kg}} \cdot \frac{1000 \text{ m}^3/\text{s}^2}{\text{kJ/kg}} \right]^{1/2} = 2735 \text{ m/s}$$

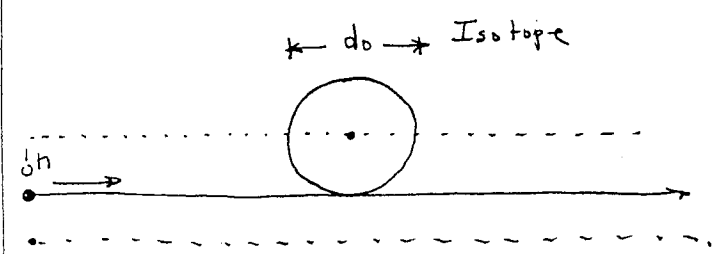
$\Rightarrow$ These neutrons are in thermal equilibrium with the environment.

Energy for one $\text{^1}_0\text{n} = \frac{1}{2}mv^2$

$$\frac{1}{2} \cdot 1 \text{ AMU} \cdot \left[\frac{2735 \text{ m}}{\text{s}} \right]^2 = 6.21 \text{ E-21 J} = 3.9 \text{ E-8 MEV}$$

- These are called "thermal neutrons" because they are in thermal equilibrium with the environment.
- Neutrons generated by fission are typically $> 0.1 \text{ MEV} \approx \frac{0.015 \text{ C}}{4.5 \text{ E+6 m/s}}$
- The Kicker: Collision ~~with~~ between U-235 + thermal $\text{^1}_0\text{n}$ is $\sim 450\times$ more likely to cause fission than with fast neutron.
- $\Rightarrow$ Imbalance between what you need and what you make
- $\Rightarrow$ Use moderator to slow $\text{^1}_0\text{n}$ (H_2O , C, Na).

③ Cross-Sections $\rightarrow$ Key to selecting reactor materials.

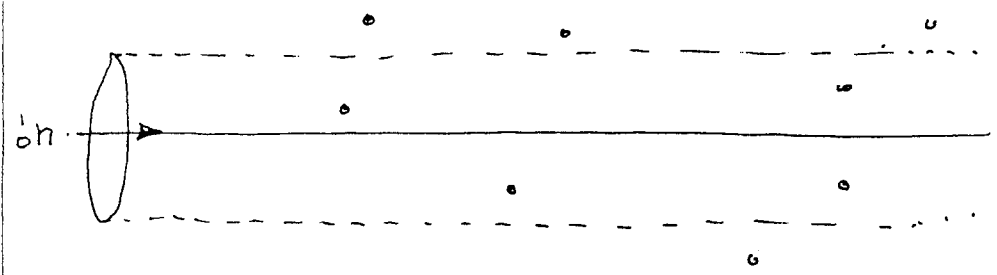


- If it passes inside circle, reaction will occur
- Outside: No.

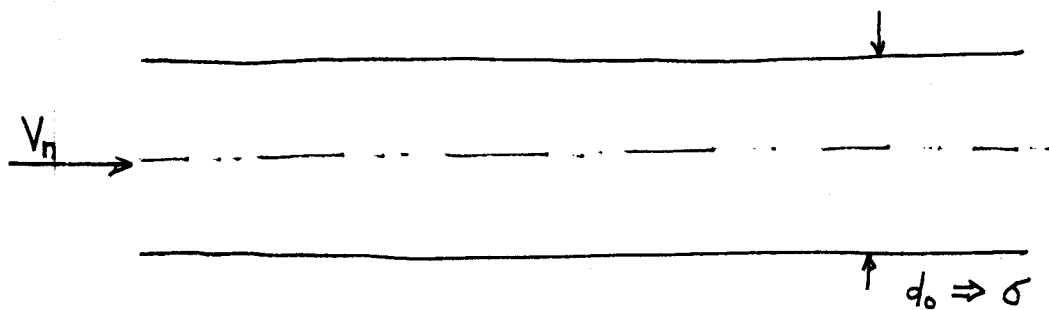
$\Rightarrow$ Can think of $\text{^1}_0\text{n}$ as having cylinder of diameter d_0 .

- In its journey, a nucleus comes inside the cylinder, then reaction will occur.
- The cross-sectional area of this cylinder ($= \frac{\pi d_0^2}{4}$) is called the cross-section
- Cross-sections vary for type of reaction, neutron speed, isotope.

$A_c = \sigma = \text{Barns} = 10^{-28} \text{ m}^2$ Bigger = more reactions

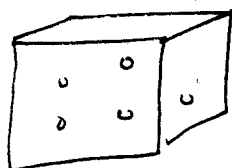


Reactions occur with any isotope inside cylinder.



1 sec: Volume Swept = $\sigma V_n = m^2 \cdot \frac{m}{s} = \frac{m^3}{s}$

1 sec: Interactions = isotopes in volume



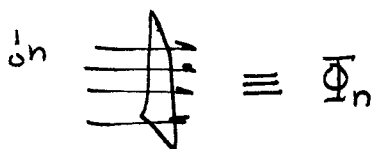
$$n_u = \frac{\text{isotopes}}{m^3} \Rightarrow \frac{\text{Interactions}}{s} = \sigma V_n n_u$$

This is for one ^1_0n . Now get for all ^1_0n in volume

$\Rightarrow$ multiply by # of ^1_0n in $1 m^3 = n_n$

$$\frac{\text{Collisions}}{\text{Sec-Volume}} = \sigma V_n n_u n_n$$

but $V_n n_n = \frac{m}{s} \cdot \frac{^1_0n}{m^3} = \frac{^1_0n}{m^2 \cdot s} = \text{flux rate of } ^1_0n$



$$\frac{\text{Collisions}}{\text{Sec-Vol}} = \sigma \Phi_n n_u \Rightarrow \text{makes sense: } \text{Flux}$$

reaction rate = $[^1_0n \text{ flux}] \times [\text{isotope density}]$

Three types of collisions:

(a) Scattering: ^1_0n absorbed and re-emitted, but are slowed down

$$\frac{\text{Scat}}{m^3 \cdot s} = \sigma_s \Phi_n n_u$$

Scattering cross-section (moderators have big σ_s)

(b) Capture: $\frac{\text{Capture}}{m^3 \cdot s} = \sigma_c \Phi_n n_u$

$\rightarrow$ Control rods

$\rightarrow$ Breeding.

(c) Fission: $\frac{\text{Fission}}{m^3 \cdot s} = \sigma_f \Phi_n n_u$

$\rightarrow$ U-235
Pu-239

Look at cross-sections of important materials. for thermal neutrons ($\sim 2700 \text{ m/s}$)
 $\sigma = \text{Barns}$.

Isotope	σ_f	σ_c	σ_s	
^1_1H	0	0.33	38	• Good moderator • Also good coolant • Some $\sigma_c \Rightarrow$ need to enrich to overcome
^2_1H	0	0.00053	7	• Fair moderator • No capture $\rightarrow$ can be used with <u>natural uranium</u> (Canada). • Coolant.
^3_2He	0	0.007	1.4	• British gas-cooled reactors. • μ low
B	0	760	4	} Control rods
B-10	0	3837	4	
C	0	0.0036	4.8	• Moderator
Na	0	0.53	4.0	• Moderator/Coolant.
U-235	584	98	10	• Fuel
U-238	0	2.71	8.3	• Fertile isotope $\Rightarrow$ New fuel
PU-239	742	270	9.6	• Fuel

For Fast $\dot{n}$ (1.5 MEV = 6% of C)

U-235	1.28	0.078	4.5	} $\sim 400\times$ decrease in reactivity.
PU-239	1.95	0.04	4.8	

Typical Population balance for 1000 ($\dot{n}$)



Nov. 9

Start
1000 fast ^1_0n

→ 130 leak

→ 4 $^1_0n + {}^{235}_{92}\text{U} \rightarrow {}^{236}_{92}\text{U}$ (lost), (fast capture)→ 26 $^1_0n + {}^{235}_{92}\text{U} \rightarrow \text{fission} + 2.5(^1_0n) \Rightarrow$ 65 neutrons.
(Fast fission)→ 120 $^1_0n + {}^{238}_{92}\text{U} \rightarrow \dots \rightarrow {}^{239}_{94}\text{Pu}$ (Breeding)

→ 10 lost to other materials (inert capture)

710 Reach
Thermal Energy

→ 27 leak

→ 72 $^1_0n + {}^{235}_{92}\text{U} \rightarrow {}^{236}_{92}\text{U}$ (lost to fuel capture)→ 374 $^1_0n + {}^{235}_{92}\text{U} \rightarrow \text{fission} + 2.5(^1_0n) \rightarrow$ 935 neutrons.→ 196 $^1_0n + {}^{238}_{92}\text{U} \rightarrow \dots \rightarrow {}^{239}_{94}\text{Pu}$ (breeding)

→ 41 lost to other materials

1000 ^1_0n outReactor Kinetics / Control.

Very rough population balance equation.

 $\text{In} - \text{out} + \text{Source} = \text{accumulation}$

$$\sigma_f n v n_u + \sigma_d n v n_u - \sigma_c n v n_c = \frac{dn}{dt} = 0 \text{ @ steady state.}$$

Now suppose I pull the control rods out some $t=0$ 1000 $\frac{\text{neutrons}}{\text{m}^3}$ How long will it take? $\begin{cases} \text{Fast} = \text{bad} \\ \text{Slow} = \text{controllable} \end{cases} \quad t=t_1 \quad 1010$

⇒ has long power doubling time (60 s) (lies w/o danger,
 ⇒ Large changes in reactivity make delayed ^1_0n irrelevant, and
 prompt set the time ⇒ Prompt - Critical. (10^{-4} s).
 ⇒ Bombs/Chernobyl.

Role of Delayed δn .

99% Prompt path: $\delta n \rightarrow \text{fission} \rightarrow 2[\delta n] \quad \tau^* = 10^{-14} \text{ s}$
 $\text{fast } \delta n \rightarrow \text{slow } \delta n \Rightarrow \tau^* = 10^{-6} \text{ s}$
 $\text{thermal } \delta n \rightarrow \text{absorbed or captured or fission: } \tau^* = 10^{-4} \text{ s}$
 $\Rightarrow \text{characteristic turnover time} = 10^{-4} \text{ s}$

1% Delayed path: $\delta n \rightarrow \text{fission} \rightarrow \text{delayed } \delta n \quad \tau^* = 30 \text{ s.}$
 $\text{delayed } \delta n \rightarrow \text{captured or fission: } \tau^* = 10^{-4} \text{ s}$
 $\Rightarrow \text{characteristic turnover time} = 30 \text{ s.}$

Think about two scenarios: $n_i = 1000 \frac{\text{neutrons}}{\text{m}^3} \xrightarrow{\text{Fission}} 2000/\text{m}^3 \xrightarrow{\text{Capture}} 1000 \Rightarrow n_f = 1000$

- 1) ~~Pump~~ Pull rods out a little $1000 \rightarrow 2000 \text{ Capture} - 990 \Rightarrow n_f = 1010$ | One generation
- 2) Pull rods all the way out $2000 \rightarrow 2000 \Rightarrow n_f = 2000$.

$$\text{growth rate} = \frac{\text{Increase in } \delta n \text{ for one generation}}{\text{average time for one generation.}}$$

$$\text{avg. time} = [0.99][10^{-4}] + [0.01][30] = 0.30 \text{ sec.} = \tau^*$$

$$\frac{dn}{dt} = \frac{n_i - n}{\tau^*} = \frac{n \left[\frac{n_i}{n} - 1 \right]}{\tau^*} = \frac{n[k-1]}{\tau^*}$$

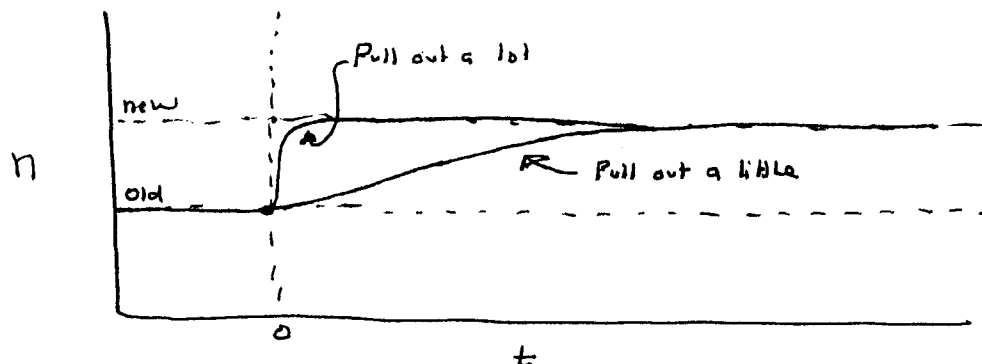
$$\text{so } n = n_0 \exp \left[\frac{t}{\tau^*/(k-1)} \right] \quad \begin{array}{l} k-1 > 0 \text{ growth} \\ k-1 < 0 \text{ decay} \end{array}$$

$$\frac{\tau^*}{k-1} = \text{time constant.} = \frac{0.30 \text{ s}}{1.01-1} = 30 \text{ seconds.}$$

$\Rightarrow$ Slow enough to be mechanically controlled δ

Case 2:

if $k=2$ time const = 0.30 s $\Rightarrow$ difficult to control.

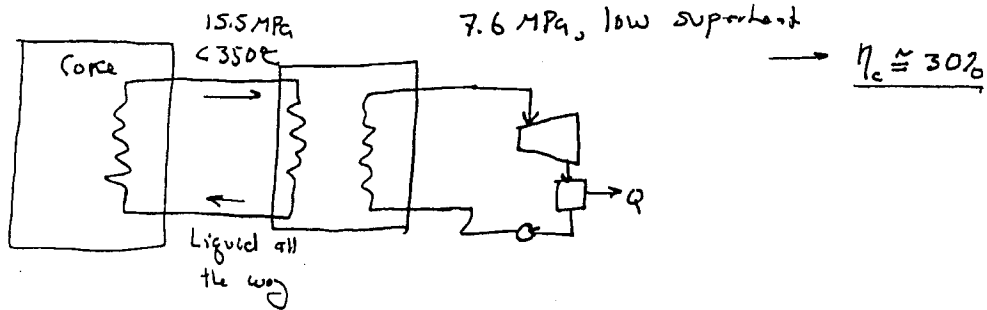


If no delayed $\text{on} \rightarrow \gamma^* = 10^{-4} \text{ s}$

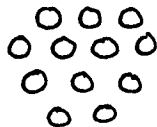
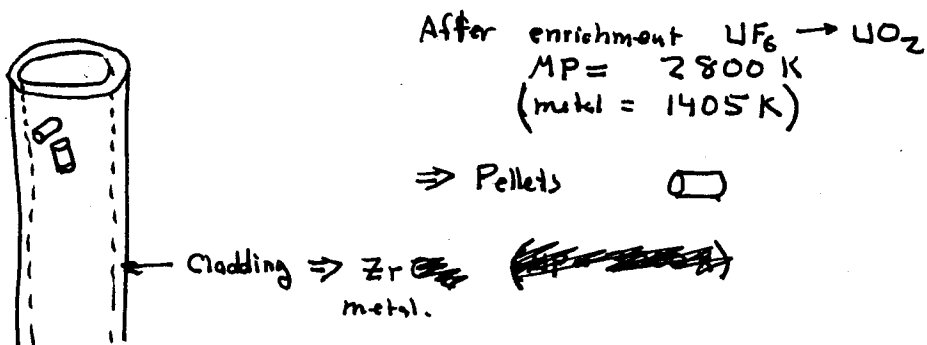
$$\text{time constant} = \frac{\gamma^*}{K-1} = \frac{10^{-4}}{1.01-1} = \text{~~10~~ } 0.01 \text{ s.}$$

Principal Reactor Systems.

① Light water reactors (US)



- Water acts as
 - coolant
 - control
 - moderator
- Fine control via boron rods
- Negative void coefficient: lose H_2O ~~and~~ → lose moderation → shuts down

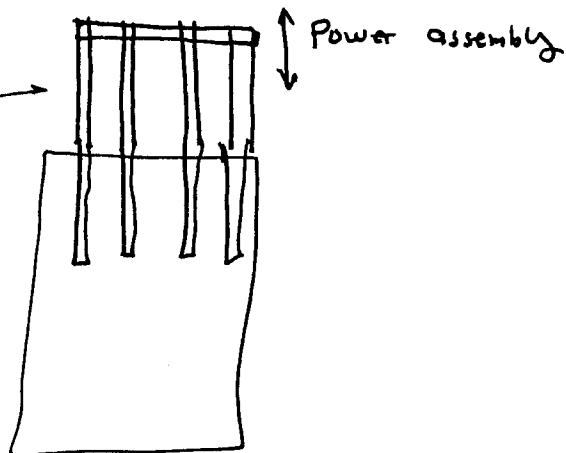


Core = hexagonal array of fuel rods.

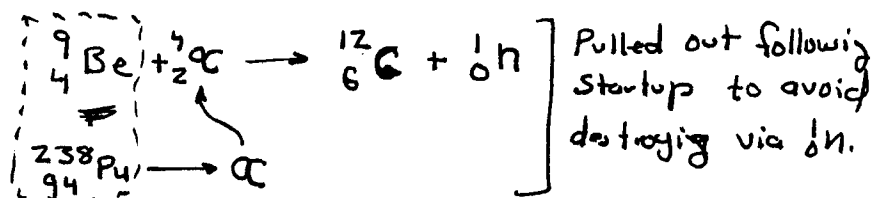
Coolant circulates over outside

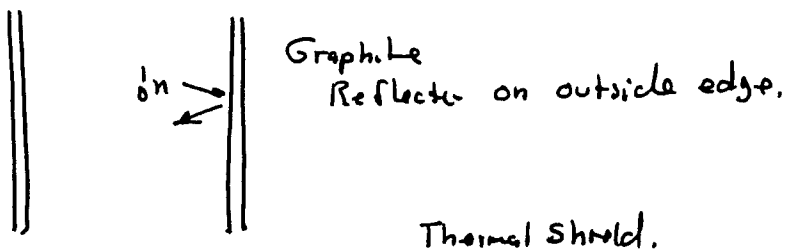
Control Rods

B_4C



Neutron source (match)



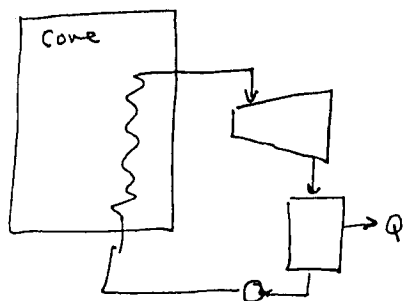


② Heavy Water Reactor (CANDU - Canada)

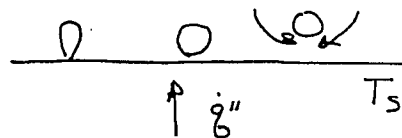
- Similar to above, but use H_2O with ${}^3H$ as coolant.
- ${}^3H$ has no capture $\rightarrow$ can run on natural U without enrichment.
 $\rightarrow$ No foreign dependency
 $\rightarrow$ Must make heavy water.
- Also negative void coefficient $\rightarrow$ safe.

③ Boiling Water Reactors

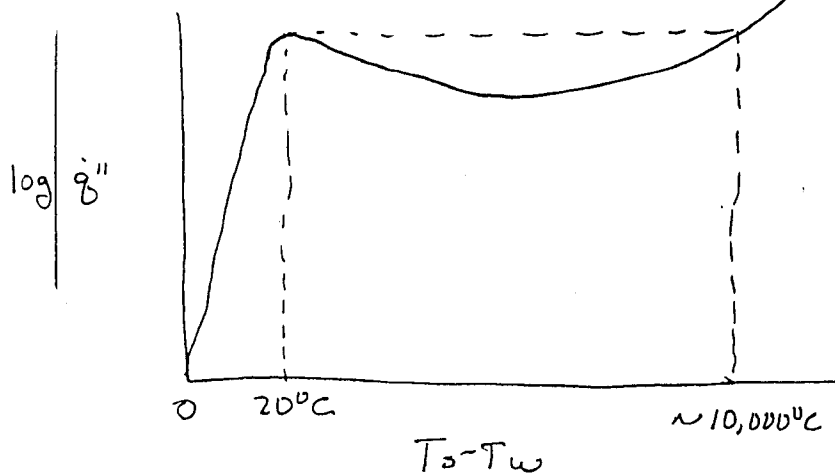
Mechanism of Boiling:



T_w (fixed).



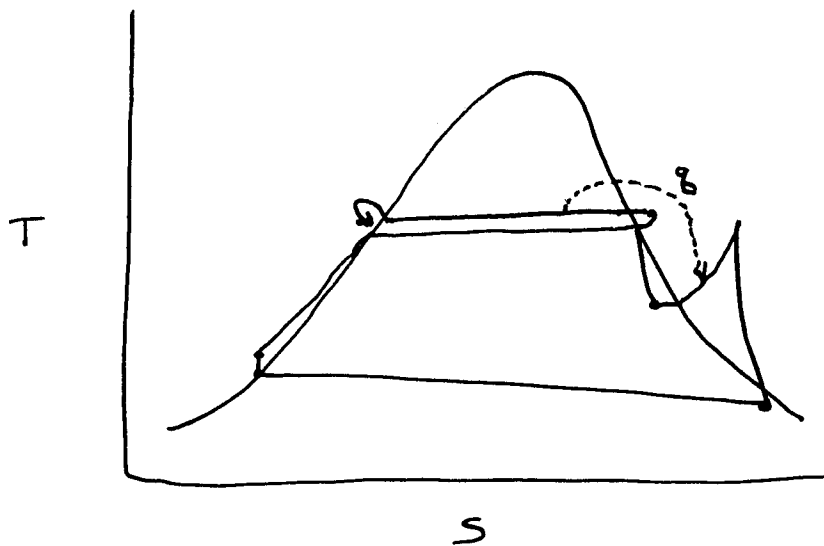
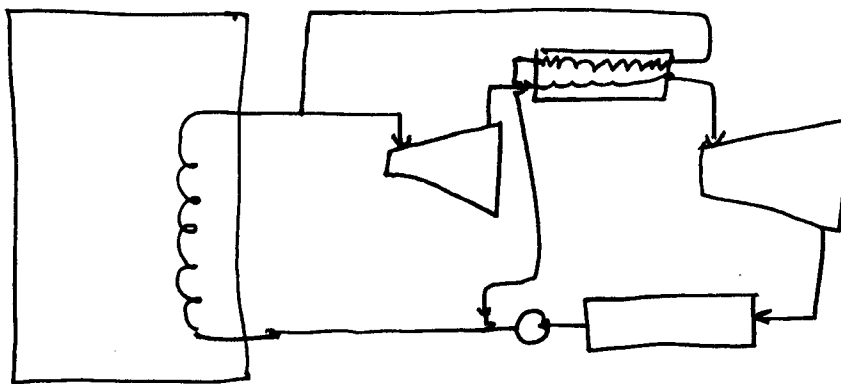
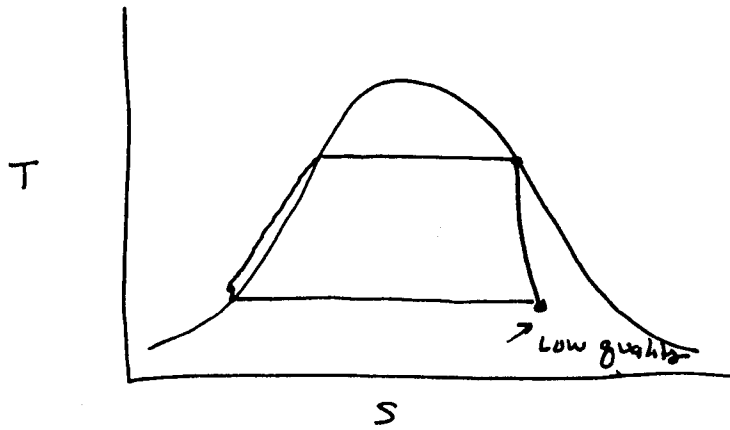
Mechanical Stirring



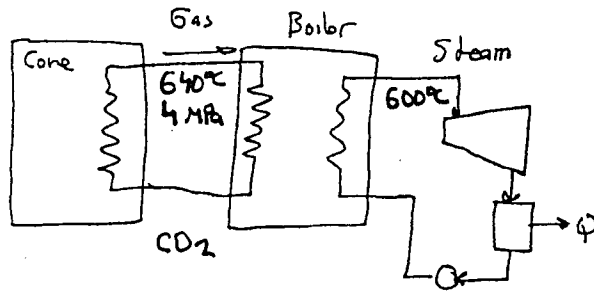
- $\Rightarrow$ Boiling is safe
- $\Rightarrow$ Superheating much more difficult to control

$\frac{1}{2}$

One main problem with low ~~power~~ superheat is wet steam in turbines:



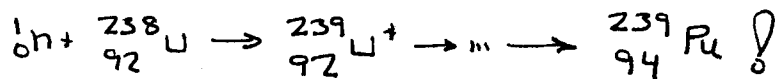
4) Gas-Cooled - British.



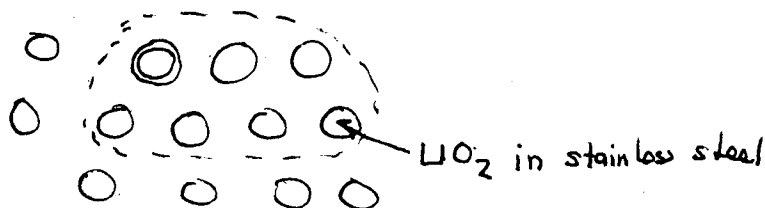
- Core is non-metal and can be run very hot. (No ΔP)!
- High superheat possible → ~~very~~ more efficient ($\eta_c = 38\%$).
- Graphite moderated → large mass, no meltdown possible. 40%
- CO₂ or He coolant.

⑤ Fast breeder reactors.

→ ~~Fast~~ $\rightarrow$

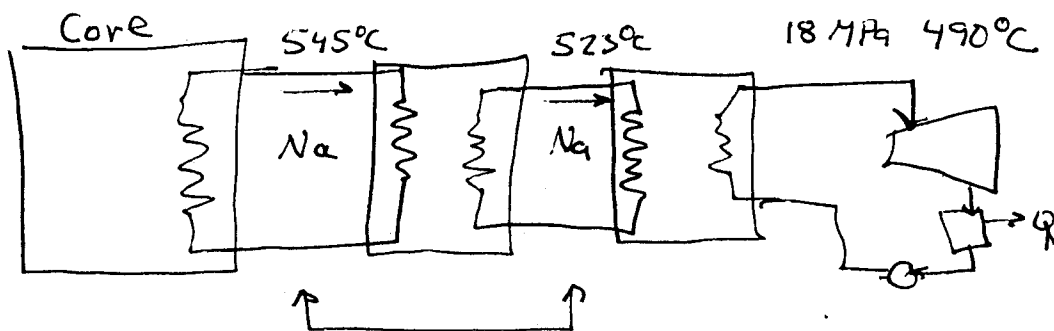


- Fast ^1_0n tend to promote breeding. [no moderator]
- But U-235 fission much slower
 $\Rightarrow$ Solution: Enrich to 15-30% rather than 3-5%.
- Use liquid Na as coolant $\Rightarrow$ low moderation -



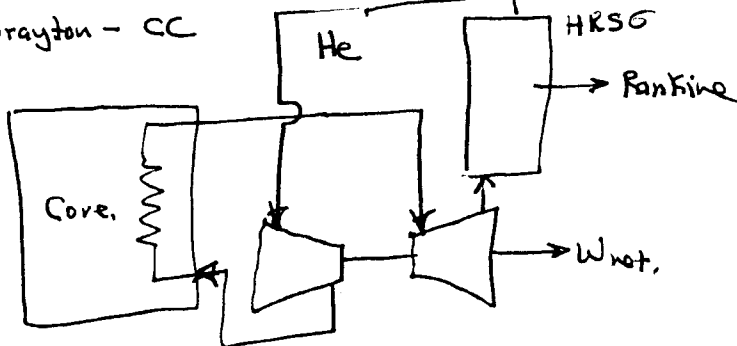
Surround with "blanket" tubes with depleted UO_2 (U-238).

Doubling time $\Rightarrow$ 10 yrs to double fuel content.



- Na becomes radioactive, so two loops needed to isolate.
- Na boils @ $\sim 900^\circ\text{C}$, so no pressurization needed,
- Huge thermal conductivity means good HT.

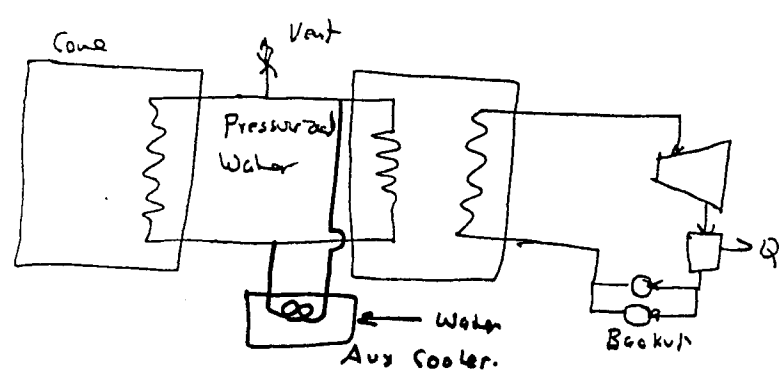
⑥ Brayton - CC



$\sim 48-50\%$

Reactor Accidents :

① Three mile island. → Light Water - pressurized.



Sequence:

- Problem caused feedwater pump to trip.
- Backup pump started
- ⇒ But: Block valves in backup line had been shut.
- No cooling load on primary water.
 - Pressure rises, causing relief valve to vent.
 - Trips reactor, inserts control rods
- But: Relief valve never closed (control panel said it did)
 - ⇒ lost all coolant.
 - (should have retained most coolant and run via aux cooling)
- Reactor was tripped, but off isn't off due to residual radioactive decay.

1000 MWe = 3333 MW thermal in operation

Shutdown ⇒ 200 MW thermal

1 day 16 MW

5 days 9 MW

⇒ This resulted in a core melt, but little release due to containment.

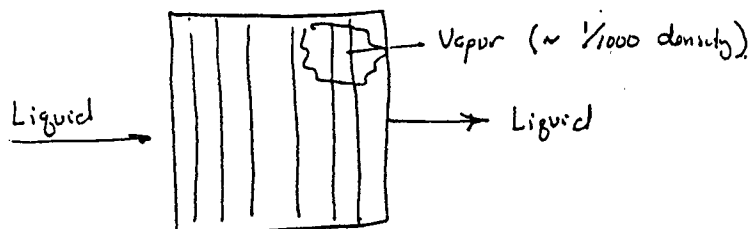
Nov. 15

Chernobyl ⇒ More complex.

→ Graphite moderated } Creates what is known as a positive void coefficient. Enough moderation, so H₂O role is captive.

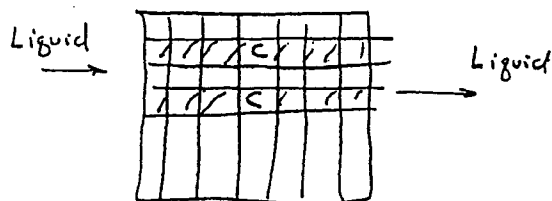
→ Light water-cooled.

- Normal reactor (US). Water moderates



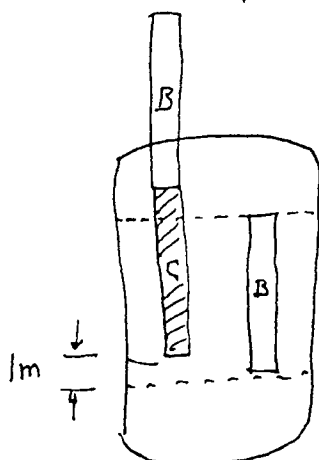
If you form a vapor pocket, locally lose moderation, and fission shuts down

- Graphite reactor:



- Graphite moderates, but control is ~ zero.
- Water moderation function is overshadowed, but control important.
 - ⇒ If you form steam packet, lots of moderation still, but lose control ⇒ reactor speeds up, ⇒ more steam
 - ⇒ Unstable. (more so @ low power).

- Emergency shutdown, drop all rods.
- Rod design problem:



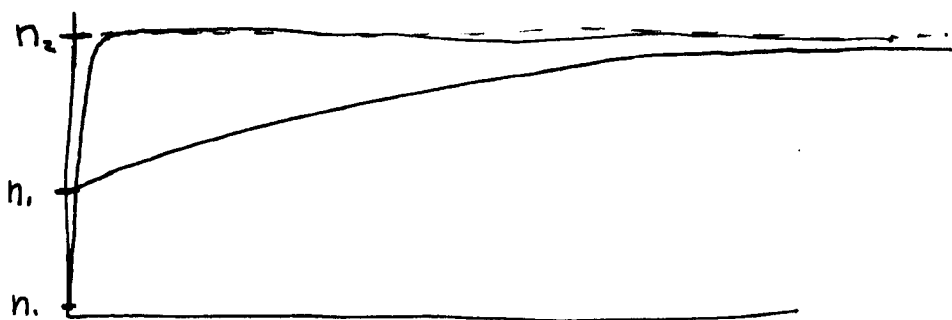
Out: Cap rod with graphite to prevent rod volume from being occupied with H_2O - a poison

In: All boron

But: $\sim 1\text{ m}$ gap @ bottom.

- When rods were pulled in, immediate response was to replace H_2O with C $\rightarrow$ more reactive

Now remember, time constant for $n_1 \rightarrow n_2$ depends on $\frac{n_2}{n_1} \Rightarrow$ large ratio $\Rightarrow$ short time



- $\Rightarrow$ First push makes reactor more reactive
- $\Rightarrow$ Normally not a problem
- $\Rightarrow$ But now gave huge n_2 , short τ] $\Rightarrow$ 100x power in 0.1 s.
 - Steam blew off top of graphite pile.
 - Graphite buried: 8 of 140 tons of fuel released.
- $\Rightarrow$ Entombed.

Prospects for nuclear:

- ~ 20% of electrical here; ~ 80% in France.
- All built in fairly short period
 - Competing designs, no standardization
 - No opportunity for operating experience to feed back into design
- Costs are very high, leadtime is ~ 15 years, if ever, politically impossible.
- Waste issue.
- Role? No CO₂ and grid-type power possible.

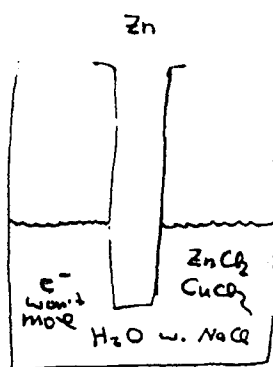


Fuel Cells

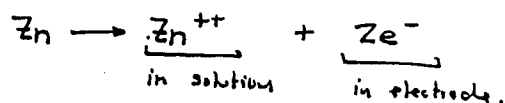
A battery with external reagent supply —
Overview — Five types:

H ₂ only (CH ₃ OH a little)	Proton Exchange Membrane (PEM)	~ 80°C	→ Lots of current work
	Alkaline	~ 100°C	→ No U.S. Activity
	Phosphoric Acid	~ 200°C	→ Commercially space programs Not much current.
	Molten Carbonate	~ 600°C	} Direct CH ₄ use. → Good hot waste heat for bottoming cycles or co-gen.
	Solid Oxide	~ 1000°C	

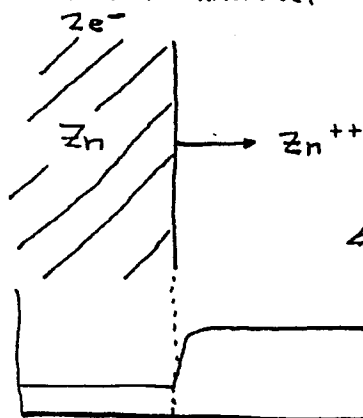
Quick overview of electrochemistry:



- Gibbs energy change for following reaction is negative (i.e., favored)



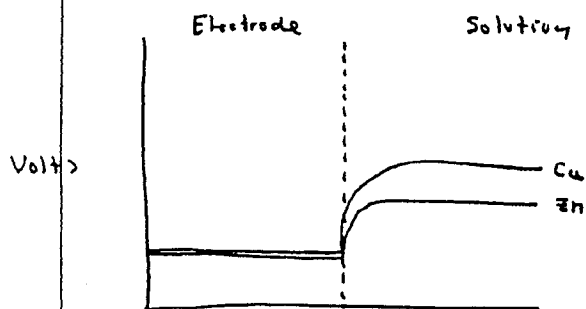
- Look at interface.



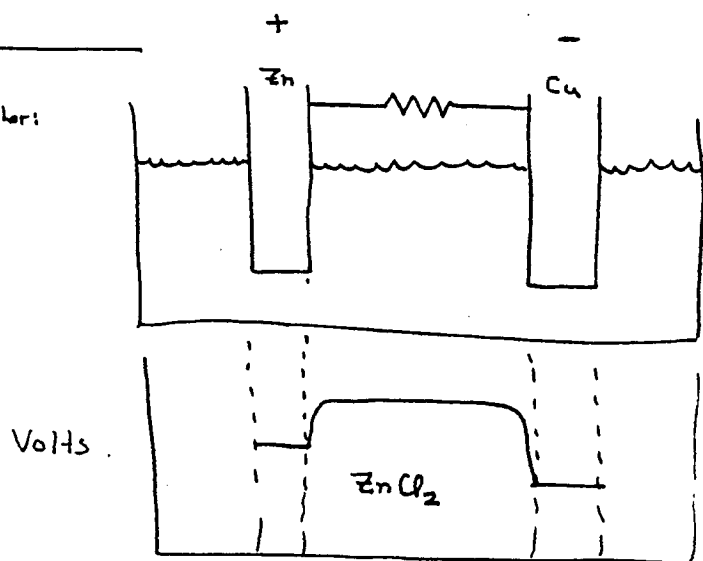
- But accumulation of "+" charge in solution and "-" change in electrode set up differential

- An equilibrium is reached in which chemistry pushing Zn into solution is balanced by charge differential

Now repeat for Cu: $\rightarrow \text{Cu}^{++} + 2\text{e}^- \Rightarrow$ Same story, but Cu chemistry is strong, it wants to be in solution more, $\Rightarrow$ Larger Voltage difference @ equilibrium



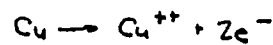
Now put them together:



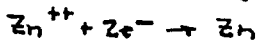
$\Rightarrow$ Since solution must be at same potential, the two electrodes will show a voltage difference.

$\Rightarrow$ Connect a load, electrons will move from "-" $\rightarrow$ "+"

Reactions @ anode (-)
@ cathode (+)

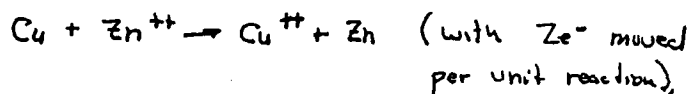


Cu into solution



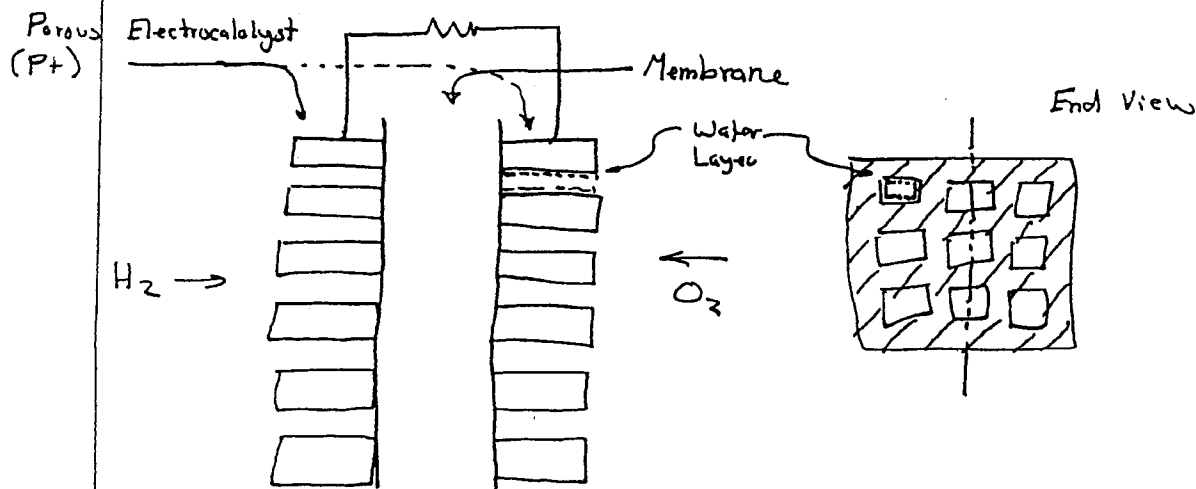
Zn plates out.

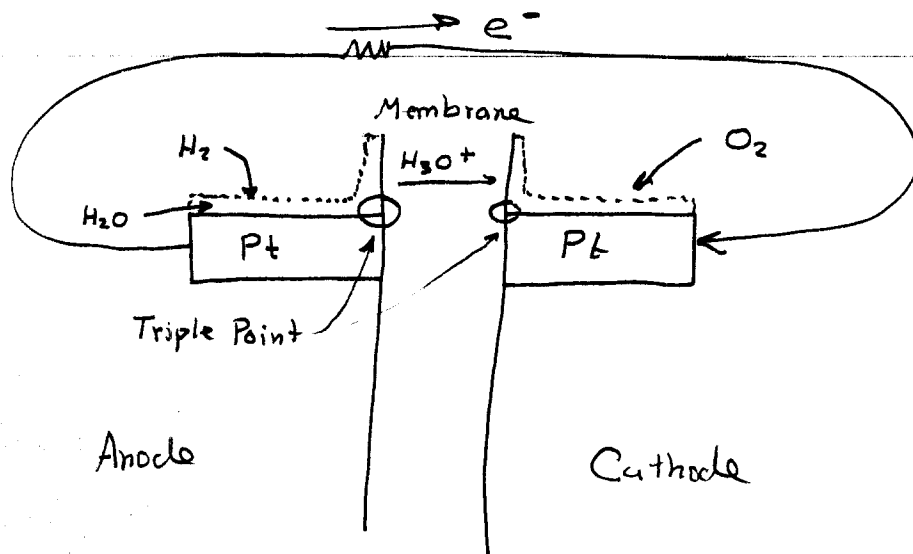
Overall



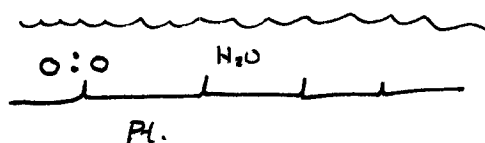
Nov 16

Now shift to simple picture of proton exchange membrane (PEM) fuel cell,





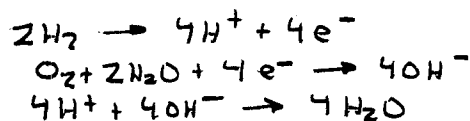
- H_2 diffuses into pores.
- H_2 dissolves in water.
- H_2 diffuses to near triple point
- $H_2 \rightarrow 2H^+ + 2e^-$



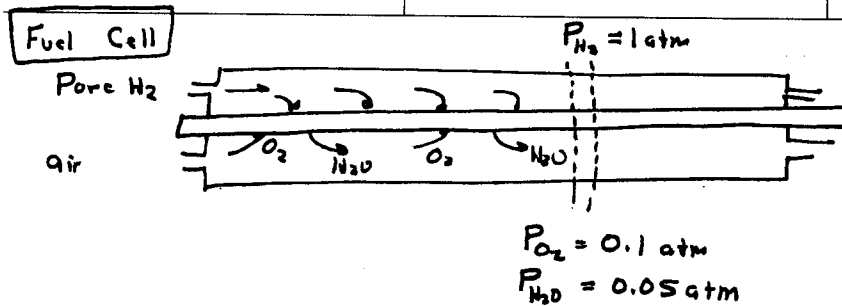
- Pt defects allow more electron mobility.
- Protons stay in liquid, e^- go into metal.

- Must be unreactive

- Membrane permiable to $H^+ \Rightarrow H^+ + H_2O \rightarrow H_3O^+$ is what goes across.
 $\rightarrow$ Membrane will only move H_3O^+ if well hydrated - wet
- At cathode: O_2 into water
- At triple points $O_2 + 2H_2O + 4e^- \rightarrow 4OH^-$
- In liquid $H^+ + OH^- \rightarrow H_2O$
- Add up reactions so e^- balance:

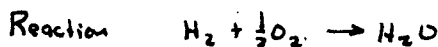


Key: Overall $2H_2 + O_2 \rightarrow 2H_2O$ [$4e^-$ moved per unit stoichiometry]



Voltage? = E

$E^0 = \frac{W_{\max}}{\text{unit charge moved.}}$



$W_{\max} = h_R - h_P - T[S_R - S_P]$

$h_R = h_{H_2} + \frac{1}{2} h_{O_2} = h_{f,H_2}^0 + [h - h_{298}]_{H_2} + 0.5(h_{f,O_2}^0 + [h - h_{298}]_{O_2})$

$h_P = h_{f,H_2O}^0 + (h - h_{298})_{H_2O}$

$S_R = S_{H_2} + \frac{1}{2} S_{O_2} = S_{H_2}^0 - R \ln \frac{P_{H_2}}{P_0} + 0.5 \left[S_{O_2}^0 - R \ln \frac{P_{O_2}}{P_0} \right]$

$S_P = S_{H_2O}^0 - R \ln \frac{P_{H_2O}}{P_0}$

$W_{\max} = h_{H_2} + \frac{1}{2} h_{O_2} - h_{H_2O} - T \left[S_{H_2}^0 - R \ln \frac{P_{H_2}}{P_0} + 0.5 \left(S_{O_2}^0 - R \ln \frac{P_{O_2}}{P_0} \right) - \left(S_{H_2O}^0 - R \ln \frac{P_{H_2O}}{P_0} \right) \right]$

$= h_{H_2} + \frac{1}{2} h_{O_2} - h_{H_2O} - T \left[S_{H_2}^0 + 0.5 S_{O_2}^0 - S_{H_2O}^0 \right] + RT \ln \left[\frac{P_{H_2} P_{O_2}^{1/2}}{P_{H_2O}} \right]$

$[W_{\max,T}]$ all species @ 1 atm

Correction for different partial pressures

$\frac{W_{\max}}{\text{kmole } H_2} \bigg| \frac{\text{kmole } H_2}{n \text{ kmole } e^-} \bigg| \frac{\text{kmole } e^-}{F \text{ coulombs}} = \frac{I}{\text{Coul}} = \text{Volts}$

$E^0 = \frac{W_{\max,T, 1 \text{ atm}}}{nF} + \frac{RT}{nF} \ln \left[\frac{P_{H_2} P_{O_2}^{1/2}}{P_{H_2O}} \right]$
 $E_{T, 1 \text{ atm}}^0 \leftarrow \text{Table!}$

Nernst Equation for rev. cell voltage.
 $= f(T, P_i)$

Quick example: 298 K

	$\frac{\text{kmole}}{\text{kmole}}$	h_f^0	$h - h_{298}$	S^0
H_2	1	0	0	130.68
O_2	0.5	0	0	205.04
H_2O	1	-241,820	0	188.83

$h_R = 0, h_P = -241,820$

$S_R^0 = 233.20 \quad S_P^0 = 188.83$

$$\begin{aligned} W_{\max, T, \text{cycle}} &= h_R - h_P - T(S_R - S_P) \\ &= 0 - (-241,820) - (298)(233.20 - 188.83) = 228,598 \frac{\text{kJ}}{\text{kmol}} \end{aligned}$$

~~Ex 12.11~~

$$E_{T, 1 \text{ atm}}^{\circ} = \frac{W_{\text{max}}}{nF} \rightarrow W_{\text{max}} = h_{\text{H}_2} + \frac{1}{2} h_{\text{O}_2} - h_{\text{H}_2\text{O}} - T \left[S_{\text{H}_2}^{\circ} + \frac{1}{2} S_{\text{O}_2}^{\circ} - S_{\text{H}_2\text{O}}^{\circ} \right]$$

$$= 0 + \frac{1}{2} 0 - (-241,820) - (298) \left[130.68 + (0.5) [205.04] - [188.83] \right]$$

$$= 228,597 \text{ KJ/Kmole H}_2$$

$$E_{T, 1 \text{ atm}}^{\circ} = \frac{228,597 \text{ KJ}}{\text{Kmole H}_2} \left| \frac{1 \text{ Kmole H}_2}{2 \text{ Kmole e}^-} \right| \left| \frac{\text{Kmole}}{9.64 \text{ E} + 7 \text{ coul}} \right| \left| \frac{10^3 \text{ J}}{\text{KJ}} \right| = \boxed{1.19 \text{ Volts}}$$

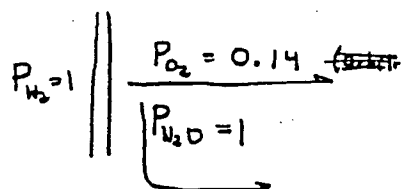
$$E^{\circ} = E_{T, 1 \text{ atm}}^{\circ} + \frac{RT}{nF} \ln \left[\frac{P_{\text{H}_2} P_{\text{O}_2}^{1/2}}{P_{\text{H}_2\text{O}}} \right] = \pi$$

$$= 1.19 \text{ Volts} + \frac{8.314 \text{ KJ}}{\text{Kmole} \cdot \text{K}} \left| \frac{298 \text{ K}}{2 \text{ Kmole e}^-} \right| \left| \frac{\text{Kmole}}{9.64 \text{ E} + 7 \text{ coul}} \right| \left| \frac{10^3 \text{ J}}{\text{KJ}} \right| \ln \left[\frac{(1)(0.1)^{1/2}}{(0.05)} \right]$$

$$1.19 + 0.0237 = \boxed{1.2137 \text{ Volts}}$$

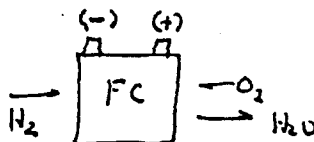
Usually the partial pressure correction is quite small, and many writers will just report the 1 atm partial pressure values. The Nernst equation, however, shows the way voltages change along a fuel cell surface as reactants are consumed and products generated.

How would picture change if H₂O was liquid?

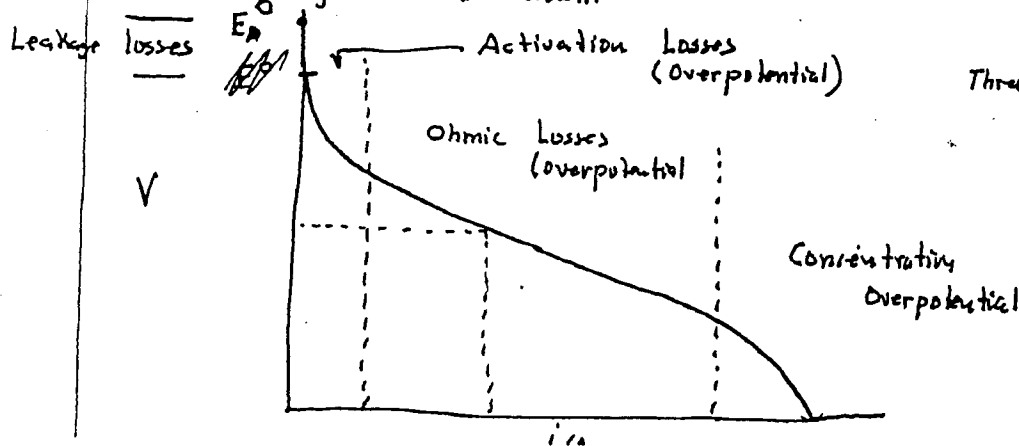


- 1) $h_{\text{F, H}_2\text{O}}^{\circ} = -285,830$
- 2) $S_{\text{H}_2\text{O}}^{\circ} = 69.92$
- 3) $P_{\text{O}_2} = 0.14$
- 4) $P_{\text{H}_2\text{O}} = 1$

This gives the voltage with no current



Like all batteries, as I start to draw current, the voltage comes down.



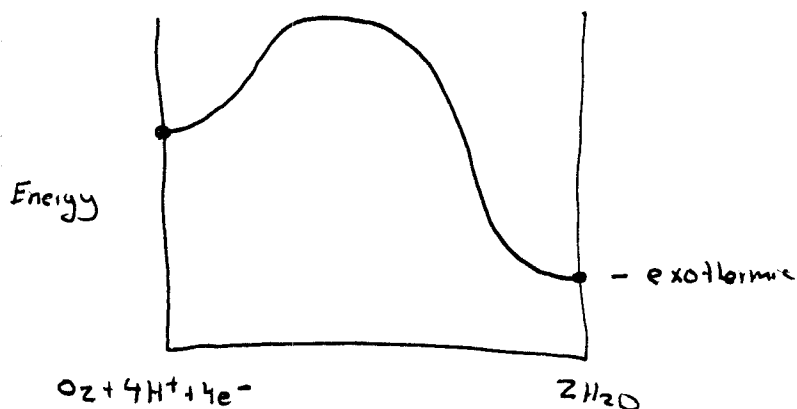
Three main effects

- ① Usually want to run where $V \times i = \text{max}$
 - ② Want to design cell to push curve to right.
- ⇒ Must understand of each of these losses.

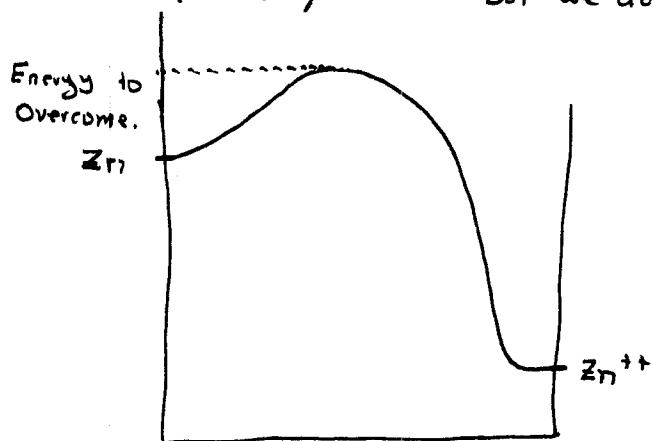
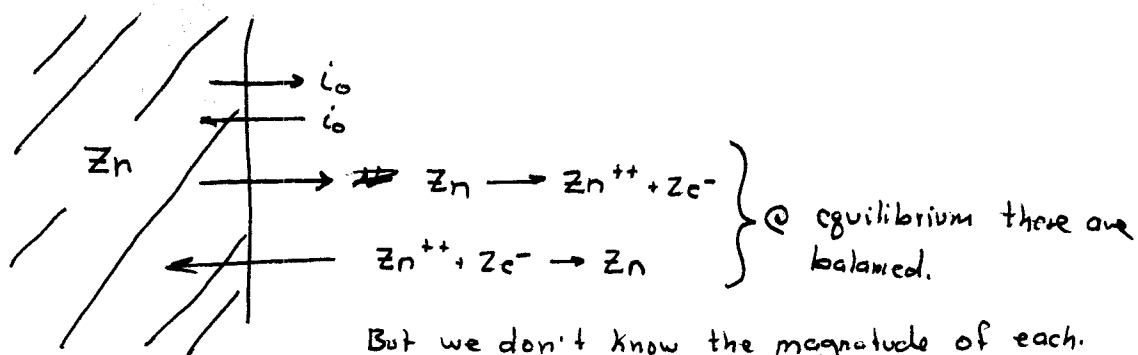
Nov 19
- Exam

Nov 21

Activation Losses: Concentrated in cathode of PEM:



Easier to see with our Zn example:

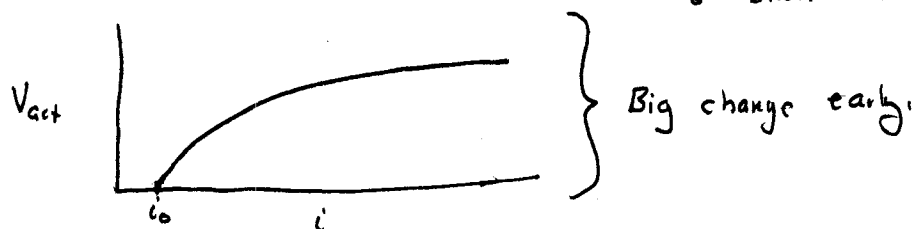


- Represent Zn flux as charge flux $= i_0$
- If energy barrier is high, i_0 is small.
- If energy barrier is low, i_0 is big.

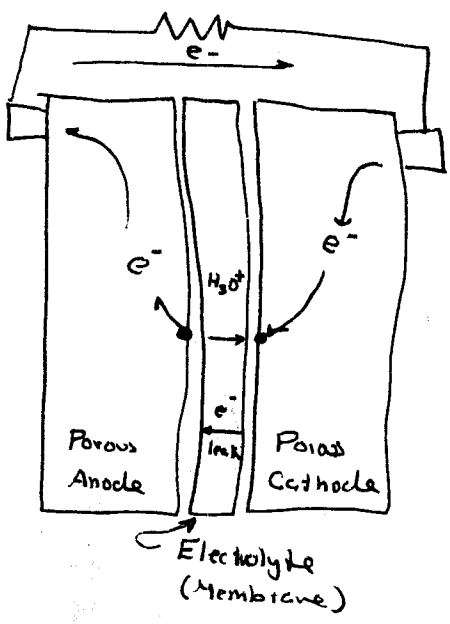
Tafel eqn semi-empirically relates these:

$$V_{act} = \frac{RT}{\alpha n F} \ln \frac{i}{i_0}$$

$$\begin{aligned}
 i &= \text{fixed} \\
 i_0 &= \text{big} \Rightarrow V_{act} = \text{small} \\
 i_0 &= \text{small} \Rightarrow V_{act} = \text{big}
 \end{aligned}$$



Resistance Losses.



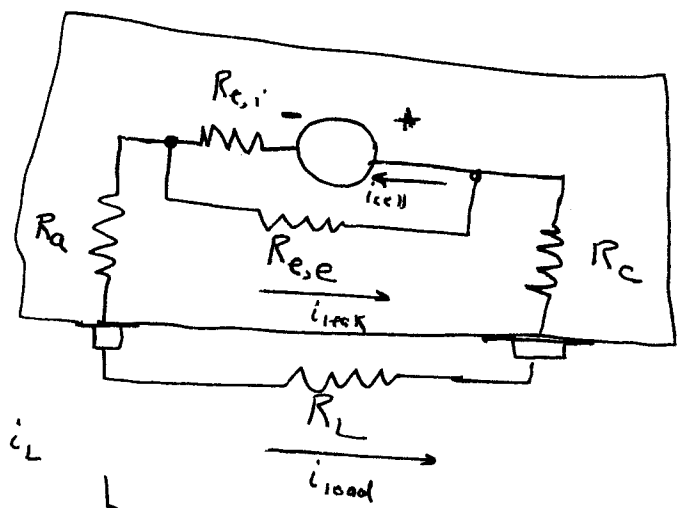
Resistances

- R_a = anode: Interconnect to reaction site
- R_c = cathode: Same
- $R_{e,i}$ = membrane for H_3O^+ flux,
- $R_{e,e}$ = membrane for e^- flux
- R_L = variable external load resistance.

Perfect design: $R_a = R_c = R_{e,i} = 0, R_{e,e} = \infty$

Equivalent Circuit:

Voltage Source = $E^0 - V_{act}$

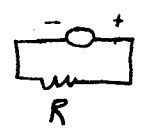


Goal: V_L vs. i_L



Some EE: Pick R_L

① Equivalent circuit is



$$R = R_{e,i} + \frac{1}{\frac{1}{R_{e,e}} + \frac{1}{R_a + R_L + R_c}}$$

$$\textcircled{2} \quad i_{\text{cell}} = \frac{E^0 - V_{\text{act}}}{R}$$

but $V_{\text{act}} = \frac{RT}{\alpha n F} \ln \frac{i_{\text{cell}}}{i_0}$

Need to iterate:

- Assume $V_{\text{act}} = 0$ to start
 - Find i_{cell}
 - Use Tafel eqn to get V_{act}
 - Kick out ~~both~~ V_{act} , i_{cell}
- ← Iterate

③ Get leak current:

$$E^0 - V_{\text{act}} = i_{\text{cell}} R_{e,i} + i_{\text{leak}} R_{e,e}$$

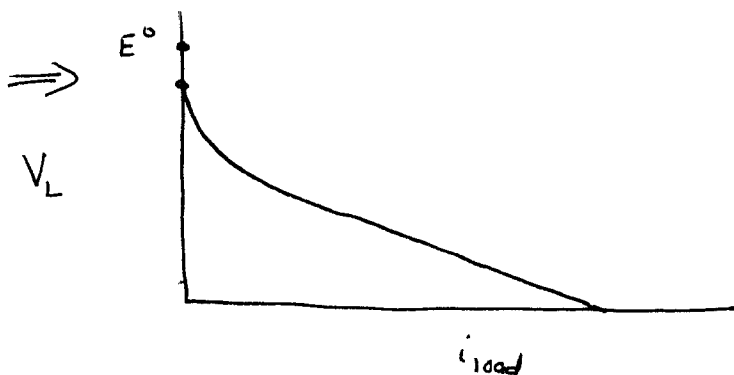
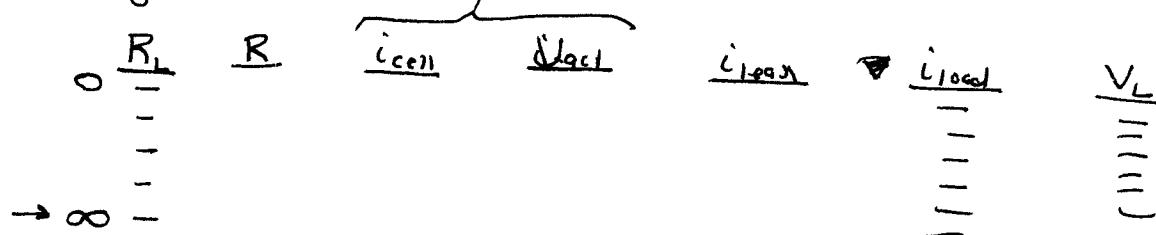
$$\text{so: } i_{\text{leak}} = \frac{E^0 - V_{\text{act}} - i_{\text{cell}} R_{e,i}}{R_{e,e}}$$

$$\textcircled{4} \quad i_{\text{load}} = i_{\text{cell}} - i_{\text{leak}}$$

$$\textcircled{5} \quad V_L = i_{\text{load}} R_{\text{Load}}$$

$$\textcircled{6} \quad P_L = V_L i_{\text{Load}}$$

So you go as follows:



Note that at $R_L = \infty$ (open circuit), still have reactant consumption.

Iterate to steady state.

So you go:

R_L

R

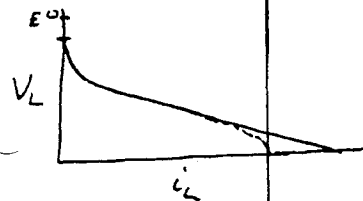
i_{cell}

V_{act}

i_{max}

i_L

V_L

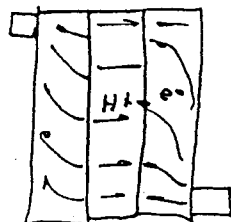


Note that $V_{act} = f(i_{cell})$, so may need to iterate.

Note that at $R_L = \infty$, still have reactant consumption.

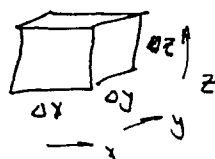
Nov 26

Now look quickly @ $R_a, R_{e,i}, R_c$ - Not intrinsic property



Non-uniform path:

Development identical to ~~Fourier~~ conduction equation + Faraday's law



$$\vec{i}_x = \frac{\text{amps}}{\text{m}^2} \text{ in } x\text{-direction}$$

Current in = current out.

$$\vec{i}_x \Delta y \Delta z \Big|_x - \vec{i}_x \Delta y \Delta z \Big|_{x+\Delta x} + \vec{i}_y \Delta x \Delta z \Big|_y - \vec{i}_y \Delta x \Delta z \Big|_{y+\Delta y} + \vec{i}_z \Delta x \Delta y \Big|_z - \vec{i}_z \Delta x \Delta y \Big|_{z+\Delta z} = 0$$

divide by $\Delta x \Delta y \Delta z$ and change sign.

$$\frac{\vec{i}_x|_{x+\Delta x} - \vec{i}_x|_x}{\Delta x} + \frac{\vec{i}_y|_{y+\Delta y} - \vec{i}_y|_y}{\Delta y} - \frac{\vec{i}_z|_{z+\Delta z} - \vec{i}_z|_z}{\Delta z} = 0$$

$$\lim \Delta x \Delta y \Delta z \rightarrow 0$$

$\sigma = \text{resistivity}$
[$\Omega \cdot \text{m}$]

$$\frac{\partial \vec{i}_x}{\partial x} + \frac{\partial \vec{i}_y}{\partial y} + \frac{\partial \vec{i}_z}{\partial z} = 0$$

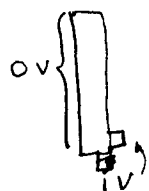
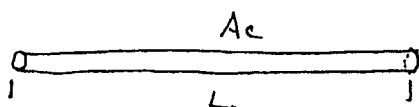
$$\frac{\partial V}{\partial x} = \sigma \vec{i}_x$$

$$\frac{\partial^2 V}{\partial x^2} = \sigma \frac{\partial \vec{i}_x}{\partial x}$$

$$\frac{\partial V}{\partial y} = \sigma \vec{i}_y$$

$$\frac{\partial V}{\partial z} = \sigma \vec{i}_z$$

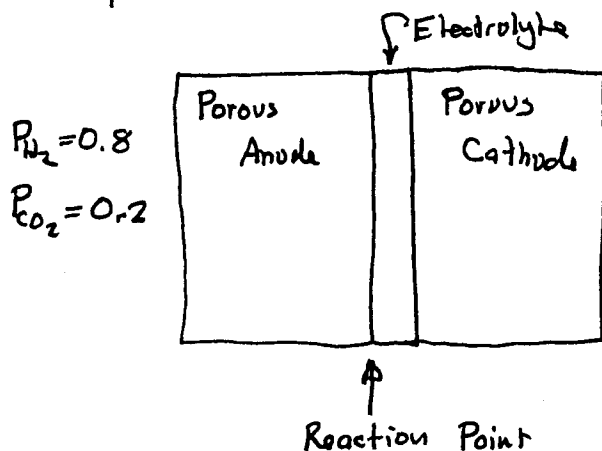
$$\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} + \frac{\partial^2 V}{\partial z^2} = 0$$



- Solve eqn for voltage field (ANSYS)
- Use gradient in field to get i @ each point
- Sum to get i
- $R_c = \frac{1V}{i}$

$$\Delta V = \frac{\sigma \cdot L}{\frac{A_c}{R}} i$$

Simple model for concentration overpotential.



• Voltage based on P_{H_2} @ reaction points not free stream.

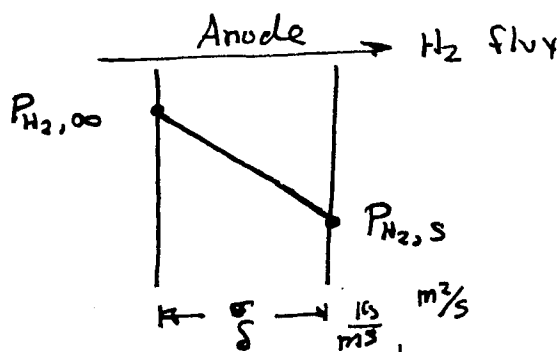
• Diffusion like heat transfer

$$\delta \sim \frac{dT}{dy} \quad H_2 \text{ Flux} \sim \frac{d(\text{mole fraction } H_2)}{dx}$$

$\Rightarrow P_{H_2}$ @ reaction point is lower.

$\Rightarrow$ Higher flux $\Rightarrow$ more P_{H_2} drops.
 $\Rightarrow$ lower P_{H_2} @ rxn.
 $\Rightarrow$ lower voltage.

Diffusion:



$$\text{flux} \sim \frac{dy_{H_2}}{dx} = \frac{[P_{H_2,\infty} - P_{H_2,s}]}{\delta P_T}$$

$$\Rightarrow \text{flux: } \frac{\text{kmol } H_2}{m^2 \cdot s} = \epsilon D \frac{P_{H_2,\infty} - P_{H_2,s}}{\delta P_T}$$

What is max possible flux? $P_{H_2,s} = 0$ [cannot draw anymore through].

$$\Rightarrow \frac{H_2 \text{ flux}}{\text{max possible flux}} = \frac{\epsilon D \frac{P_{H_2,\infty} - P_{H_2,s}}{\delta P_T}}{\epsilon D \frac{P_{H_2,\infty} - 0}{\delta P_T}} = 1 - \frac{P_{H_2,s}}{P_{H_2,\infty}}$$

or $\frac{P_{H_2,s}}{P_{H_2,\infty}} = 1 - \frac{\text{flux}}{\text{max flux}} = 1 - \frac{i_{\text{cell}}}{i_{\text{max}}}$

Nernst: $E^0 = E_T^0 + \frac{RT}{nF} \ln \left[\frac{P_{H_2,s} P_{O_2}^{1/2}}{P_{H_2O}} \right]$

for $i_{\text{cell}} = 0 \Rightarrow E^0 = E_T^0 + \frac{RT}{nF} \ln \left[\frac{P_{H_2,\infty} P_{O_2}^{1/2}}{P_{H_2O}} \right]$

$$\Delta E_{\text{conc}} = E^0 - E_{i=0}^0 = \frac{RT}{nF} \left[\ln \left(\frac{P_{H_2,s} P_{O_2}^{1/2}}{P_{H_2O}} \right) - \ln \left(\frac{P_{H_2,\infty} P_{O_2}^{1/2}}{P_{H_2O}} \right) \right]$$

$$= \frac{RT}{nF} \ln \left[\frac{P_{H_2,s}}{P_{H_2,\infty}} \right] = \frac{RT}{nF} \ln \left[1 - \frac{i_{\text{cell}}}{i_{\text{max}}} \right]$$

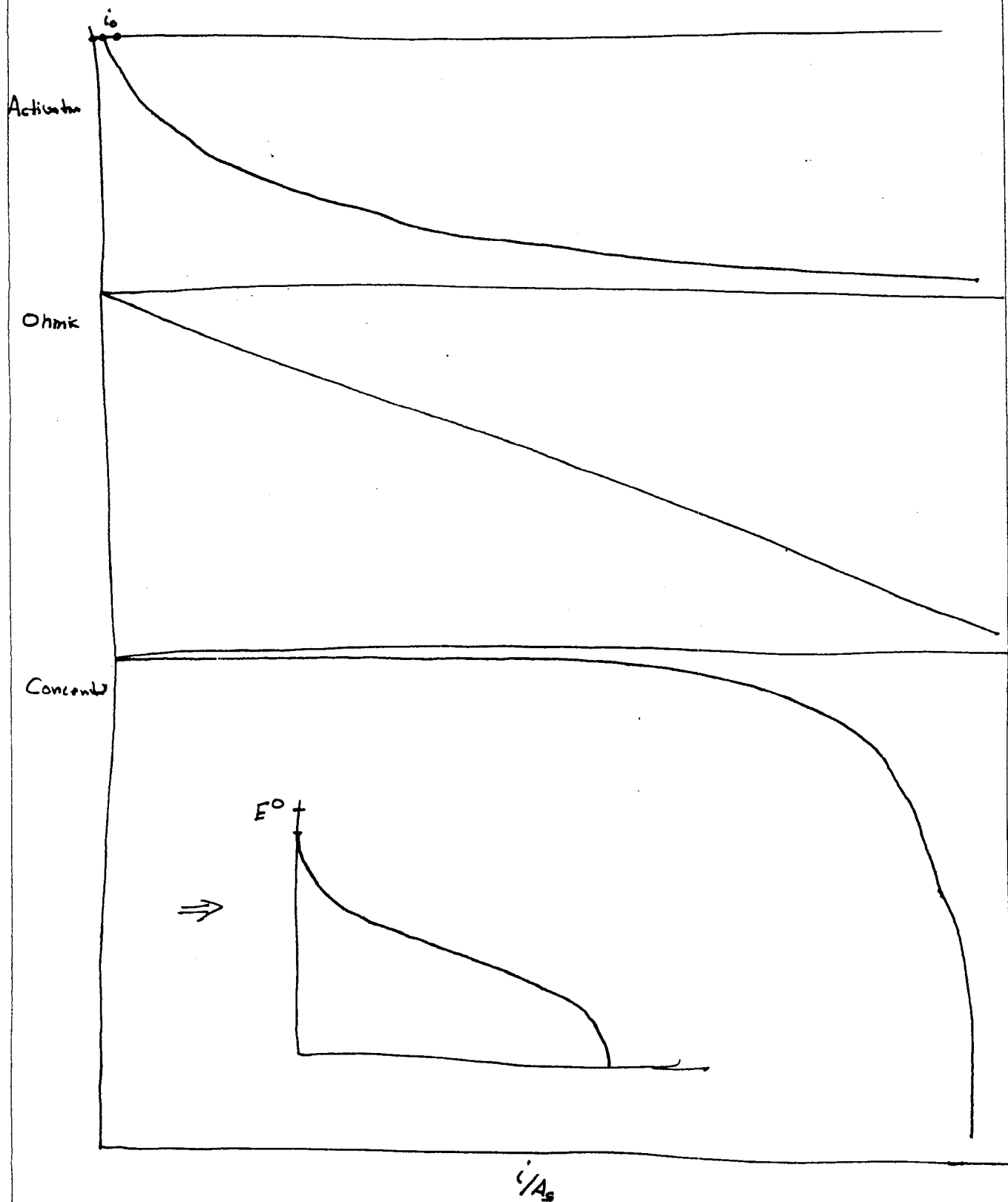
But i_{max} not realizable... why?

$$\frac{i_{\text{cell}}}{i_{\text{max}}} \quad \frac{\Delta E_{\text{conc}}}{0}$$

$$\Delta E_{conc} = E_{i \rightarrow 0} - E^0 = \frac{RT}{nF} \ln \left(\frac{P_{H_2, \infty} P_{O_2}^{1/2}}{P_{H_2, 0}} \right) - \frac{RT}{nF} \ln \left(\frac{P_{H_2, 0} P_{O_2}^{1/2}}{P_{H_2, 0}} \right)$$

$$= \frac{RT}{nF} \ln \left[\frac{P_{H_2, \infty}}{P_{H_2, 0}} \right] =$$

So Put it together:



Nov 28

Think about design:

- ① Concentration Overpotential:
 - Thin electrodes
 - Open pores.
- ② Activation Overpotential:
 - Run hot (i_0 increases with T).
- ③ Ohmic Overpotential:
 - Short current paths.
 - Thin electrolyte
 - Thick, ^{low} non-porous electrode.
 - Many current pickups.

① Start with membrane: Nafion (teflon-like polymer), 175 μm thick
big cost --- \$175/ft².

③ Bond electrodes to either side (paint).

⊙ Pt (10%).

Standard: 0.6 mg Pt/cm², 60 μm thick.

An aside - Pt demand ---

Assume a SOHP engine $\frac{\text{SOHP}}{\text{HP}} \frac{0.746 \text{ KW}}{1} = 37.3 \text{ KW}.$

 $1 \text{ cm} = 0.5 \text{ V}$
 $0.5 \text{ A} \} 0.25 \text{ W}.$

$\frac{0.6 \text{ E-3 g Pt}}{\text{cm}^2} \frac{\text{cm}^2}{0.25 \text{ W}} \frac{37,300 \text{ W}}{1} = 90 \text{ gm Pt}.$

2004 World Pt prod = 170 tons,

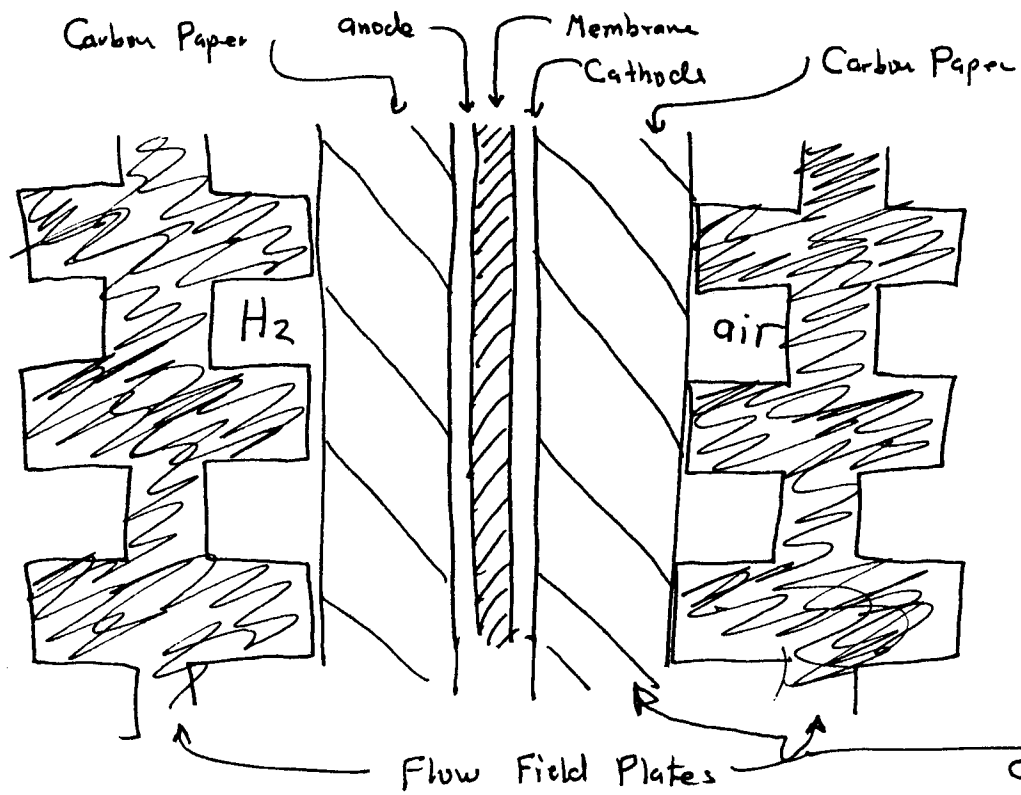
$\Rightarrow \frac{170,000,000 \text{ g}}{90 \text{ gm}} \frac{\text{Vehicle}}{\text{yr}} = 1.9 \text{ E+6 } \frac{\text{Vehicle}}{\text{yr}}$

$\Rightarrow$ Less Pt. (hurts CO resistance)

$\Rightarrow$ Thinner electrode (reduces performance).

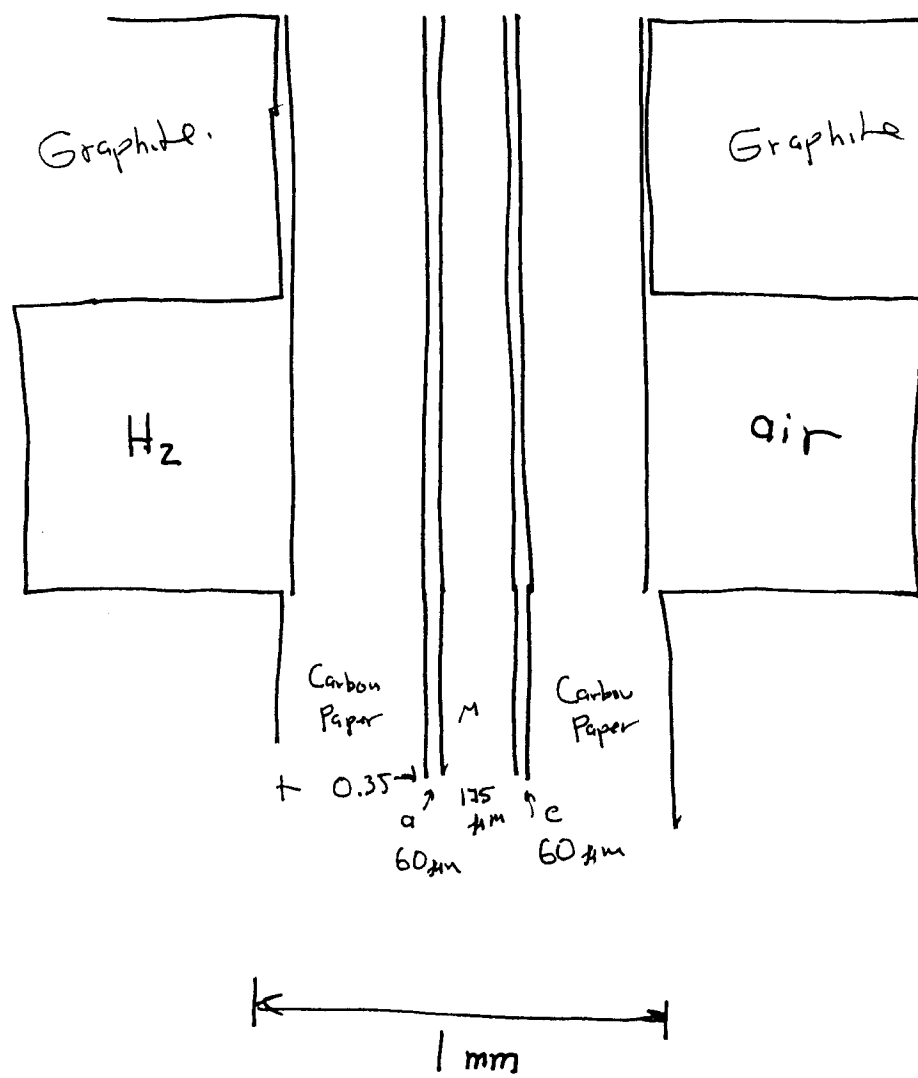
- ③ Use porous carbon paper to help distribute reagents. 0.35 mm thick
- ④ Channelled graphic flow-field plate

⑤ Plates for air : water cooling.



Why the carbon paper? Explain —

Discuss Exava



Operational Issues:

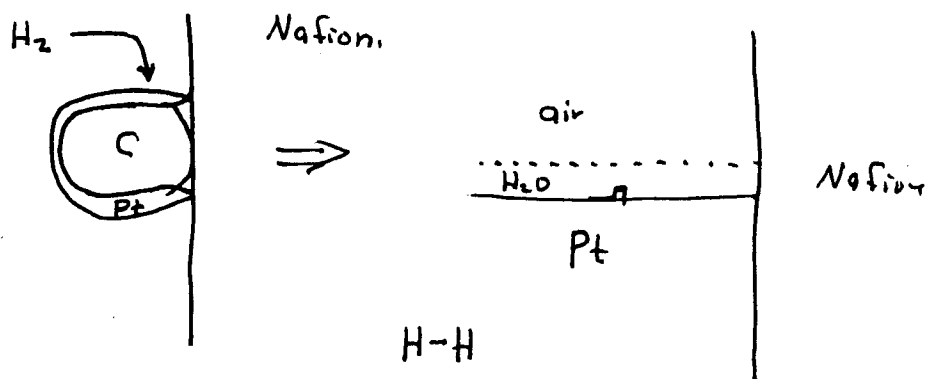
P & T Nernst: High P helps
Low T helps.

Activation: - High - T helps (i.e. up).

Membrane Conductivity: High T helps.

Pressure: Higher gas densities for small volumes, Keep some H_2O liquid
 $\Rightarrow 80^\circ C \Rightarrow$ Hot so you can run with liquid H_2O . and good membrane integrity —
 $\sim 3 \text{ atm}$

Nov. 29

CO Problem:

$H-H$

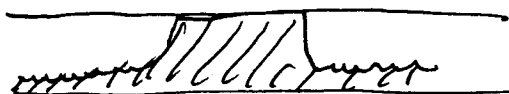
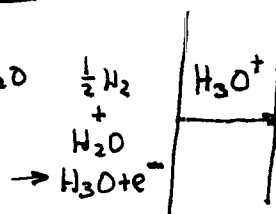
$H \uparrow H$

$\rightarrow$ Bond energy "diffused" into Pt.
 $\rightarrow$ Reduces energy needed to break
 $\rightarrow$ Pt stable, so defects are not destroyed.

- $\rightarrow$ CO adsorbs onto defects.
- $\rightarrow$ Half life for leaving long, so if y_{CO} too high, most defects will be occupied.
- $\rightarrow$ ~~At~~ At $80^\circ C$ CO < 10 ppm will leave enough sites open to allow good reactivity.
- $\rightarrow$ Higher T, more CO tolerated.

Water management:

- Membrane needs hydration
- Must humidify H_2 side to provide H_2O for H_2 passage
- Must eliminate H_2O on cathode



$\uparrow$ liquid slug has 100x the viscosity of gas $\rightarrow$ large ΔP .

H₂ Storage:

Octane: 20 gal tank:

$$\frac{20 \text{ gal}}{\text{gal}} \left| \frac{231 \text{ in}^3}{\text{in}^3} \right| \left| \frac{(2.54 \text{ cm})^3}{\text{in}^3} \right| \left| \frac{0.708 \text{ g}}{\text{cm}^3} \right| = \begin{cases} 53,601 \text{ g} \\ 118.1 \text{ lb} \end{cases} / \text{tank}$$

$$\frac{53,601 \text{ g}}{\text{g}} \left| \frac{44,430 \text{ J}}{\text{g}} \right| \left| \frac{\text{MJ}}{10^6 \text{ J}} \right| = 2381 \text{ MJ/tank.}$$

Liquid H₂ - 20 K:

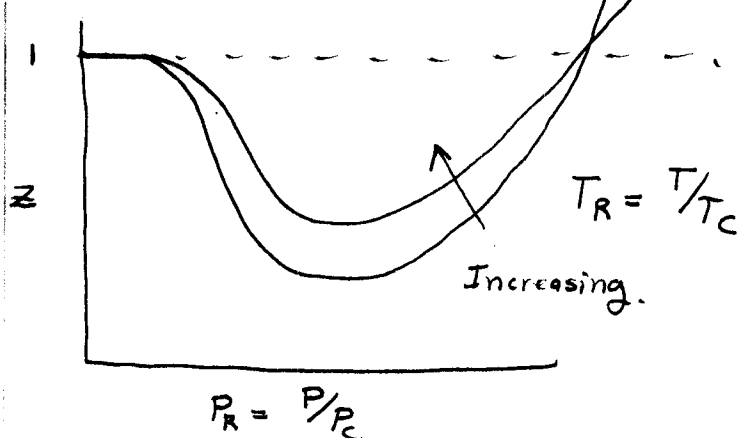
Same energy as 20 gal of octane

$$\frac{120,000 \text{ J}}{\text{g}} \left. \right\} \Rightarrow \frac{43.7 \text{ lb}}{\text{lb}} \Rightarrow \text{good mass!}$$

but $\rho = 0.07 \frac{\text{g}}{\text{cm}^3}$

$$\text{so } \frac{2,381,000 \text{ kJ}}{\text{kJ}} \left| \frac{\text{g}}{120. \text{ kJ}} \right| \left| \frac{\text{cm}^3}{0.07 \text{ g}} \right| \left| \frac{\text{in}^3}{(2.54 \text{ cm})^3} \right| \left| \frac{\text{gal}}{231 \text{ in}^3} \right| = \frac{75 \text{ gal}}{\sim 3.74 \times \text{bigger.}}$$

Pressurized? $PV = nRT$? no $PV = ZnRT$?



$$V = \frac{ZnRT}{P}$$

- So initially will occupy smaller V than V_{ic}
- Then larger due to finite volume of particles
- Liquid is like close packing

	Critical	5000 psi, 298K	10,000 psi, 298K
T	33.3 K	$T_R = 9.01$	$T_R = 9.01$
P	1.3 MPa	$P_R = 26.5$	53.0
Z		1.2	1.5
ρ		0.023 g/cc	0.037

$$\rho = \frac{P}{ZRT} = \frac{37,450 \text{ KPa}}{1.2} \left| \frac{\text{kmol} \cdot \text{K}}{8.314 \text{ KPa} \cdot \text{m}^3} \right| \left| \frac{2 \text{ kg}}{\text{kmol}} \right| \left| \frac{10^3 \text{ g}}{\text{kg}} \right| \left| \frac{\text{m}^3}{10^6 \text{ cm}^3} \right| = 0.023 \text{ g/cm}^3$$

$\Rightarrow$ Size 228 gal 143

Metal Hydrides 11,000 - 12,000 J/cm³ Octane was 31,450 J/cm³
 liquid H₂ 8400 J/cm³

⇒ Tank = 52 gal. But will hold only 5% by mass

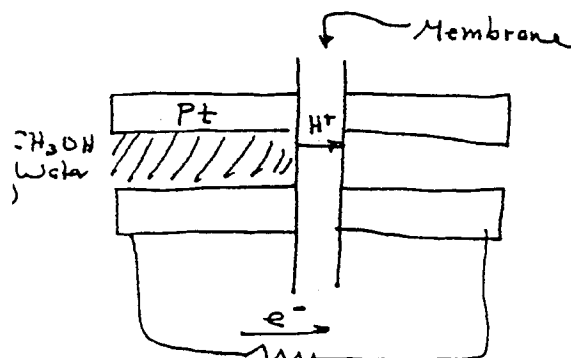
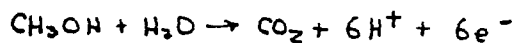
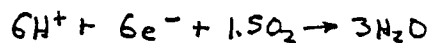
$$\frac{43.7 \text{ lb H}_2}{0.05 \text{ lb H}_2} = 874 \text{ lb.}$$

Summary:

	<u>Vol (gal)</u>	<u>mass (lb)</u>
Octane	20	118
Liquid H ₂ (20K)	74	43.7
5000 psi	228	43.7
10,000 psi	143	43.7
Hydride	52	874

Nanotubes?

Nov. 30

Direct CH₃OH PEMAnode reaction:H⁺ crosses membraneCathode reaction:⇒ CO₂ is produced @ anode⇒ H₂O produced @ cathode

⇒ System is run very wet, essentially a methanol/water solution is fuel.

⇒ Pluses:

- Liquid fuel, better energy storage than H₂ ~~for~~
- No need for reformer, get CH₃OH from biomass.

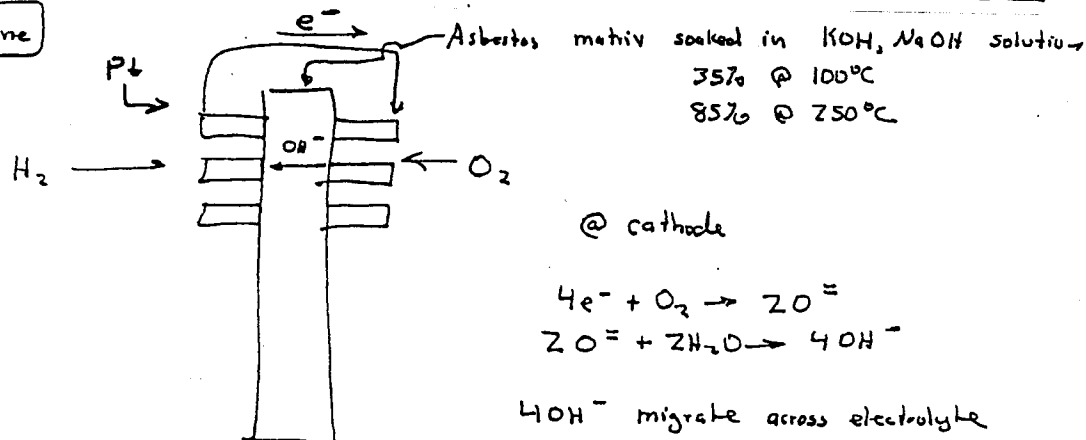
⇒ Minuses:

- Higher activation energy barrier, surface reaction rate low.
⇒ low current density

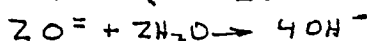
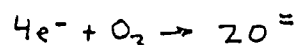
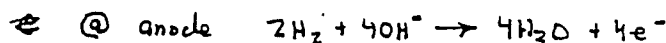
$$\text{PEM} \left\{ \begin{array}{l} \text{H}_2 = 1 \text{ amp/cm}^2 \\ \text{CH}_3\text{OH} = 0.2 \text{ amp/cm}^2 \end{array} \right\} \text{5x bigger}$$

- The usual membranes are permeable to CH₃OH
⇒ fuel crosses over and oxidizes @ cathode without making electricity.
- Lots of CH₃OH escapes the fuel side, and it must be recovered.

Alkaline



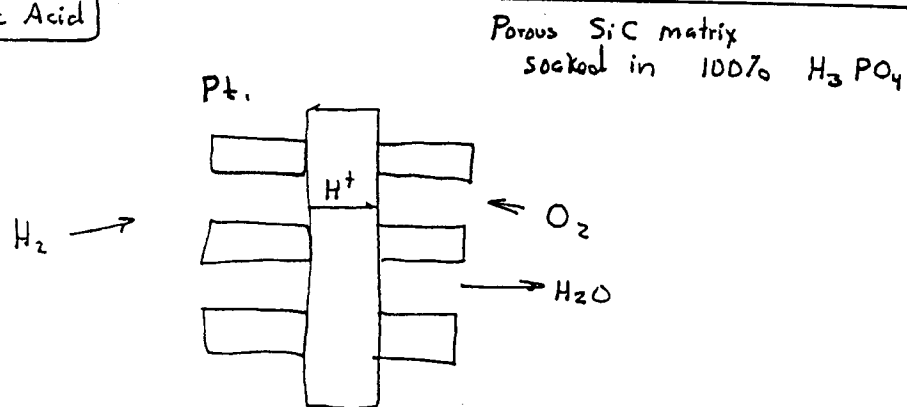
@ cathode

4OH⁻ migrate across electrolyteNotes:

- OH⁻ is ion that moves
- Water management?
 - H₂O absorbed on O₂ side, and must be supplied
 - H₂O produced on H₂ side, must be removed.
- CO is a poison
- CO₂ is also a poison $2\text{KOH} + \text{CO}_2 \rightarrow \text{K}_2\text{CO}_3 + \text{H}_2\text{O}$
- No US activity on this design.

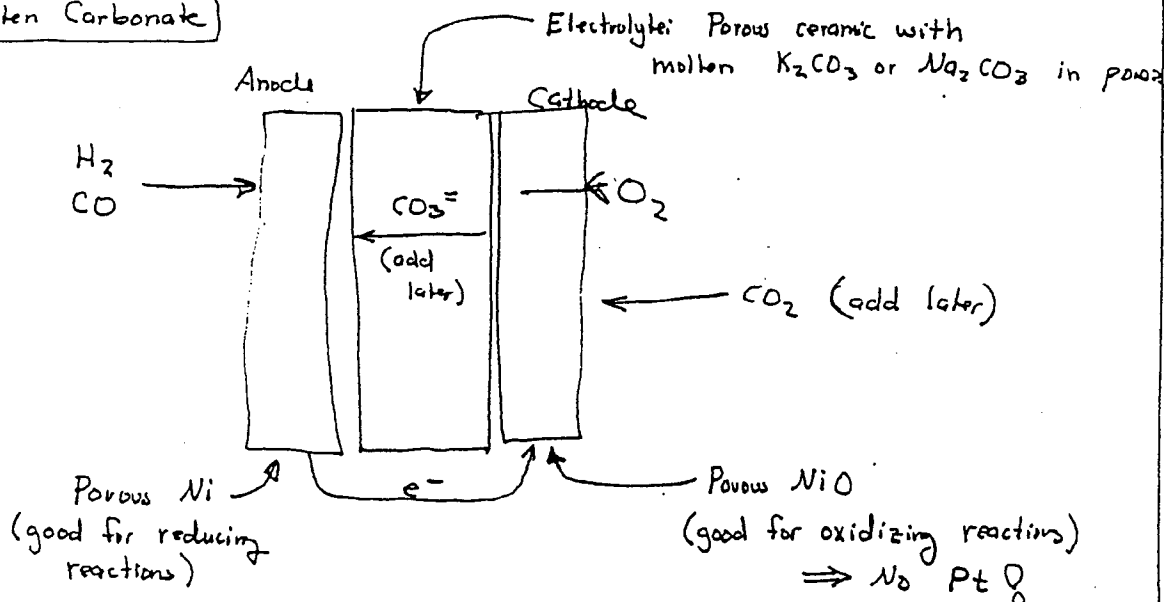
Note: Not as good as ~~DMFC~~
PEM + CO₂ poison ⇒ non-competitive

Phosphoric Acid



- Same chemistry as PEM
- 200°C , 8 atm. ~~High~~ low
- Used on Apollo spacecraft.
- Rejected heat good enough for heating.
- Electrolyte more resistive than PEM.
 $\sim 0.25 - 0.5 \text{ Amps/cm}^2$
- CO still a problem but limit is $\sim 1\%$ due to higher T.
- Been around a long time
 - Mature technology
 - Viewed with less potential for improvement than PEM
 - No real development
- One US manufacturer.

Molten Carbonate



@ cathode: $\text{O}_2 + 2\text{CO}_2 + 4\text{e}^- \rightarrow 2\text{CO}_3^-$
 $\Rightarrow$ Need to supply CO_2 to cathode

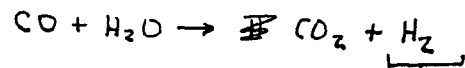
CO_3^- migrates across electrolyte

@ anode: $2\text{H}_2 + 2\text{CO}_3^- \rightarrow 2\text{H}_2\text{O} + 2\text{CO}_2 + 4\text{e}^-$

→ Direct

Two pathways for CO:

1. Direct electrolytic: $\text{CO} + \text{CO}_3^{2-} \rightarrow 2\text{CO}_2 + 2\text{e}^-$
2. Water gas shift in Ni catalyst



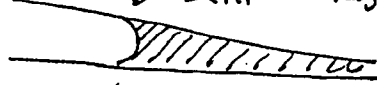
As H_2 is reacted away, equilibrium drive reaction to right, and CO is eventually drained away.

Electrolyte is corrosive and tricky.

→ Matrix is LiAlO_2

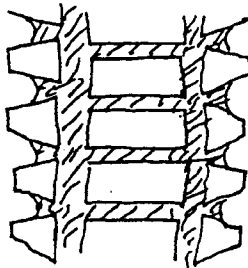
→ Use surface tension to retain electrolyte.

↓ Dcrit = largest filled diameter.



↑

Electrolyte

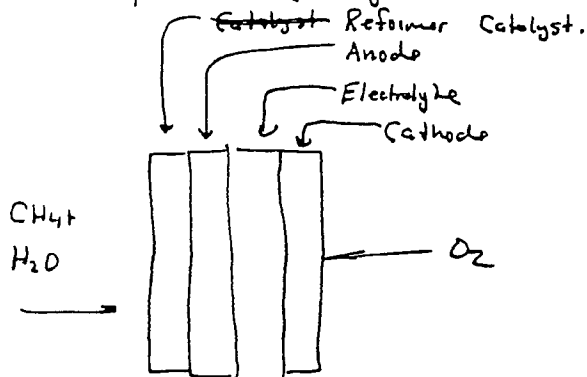


- Electrolyte pores always filled
- Tailor pore size distribution in electrodes to wet some surfaces and hold electrolyte in place.

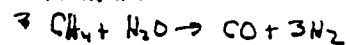
• Run @ $\sim 650^\circ\text{C}$

- Good heat for Rankine cycle
- Cool enough so standard construction materials can be used.

A neat point is the integrated internal reformer.



• In reformer:



• H_2 diffuses into electrolyte and is consumed

• CO diffuses into electrolyte and is water-gas shifted to $\text{CO}_2 + \text{H}_2$

• Reduction in CO & H_2 partial pressures drives reaction to right.
⇒ Good H_2 conversion, even @ lower T s.

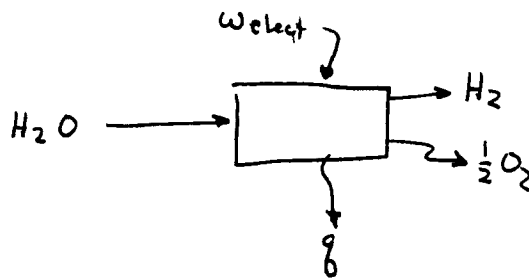
• Heat needed by steam reforming comes from cell reaction.

⇒ Nice package.

⇒ Status: R&D.

higher

Dec 3

H₂ manufacture:Electrolysis:

$$W_{\min} = h_R - h_P - T_0(S_R - S_P)$$

$$= [-285,830 - 0] - (298) [69.92 - 130.68 - 0.5(205.04)]$$

$$= -237,173 \text{ KJ/Kmole H}_2$$

$$\Rightarrow \frac{\text{KW-hr}}{\text{kg}}$$

$$\frac{237,173 \text{ KW-s}}{\text{Kmole H}_2} \times \frac{\text{hr}}{3600 \text{ s}} \times \frac{\text{Kg}}{2 \text{ Kg H}_2} =$$

$$32.9 \frac{\text{KW-hr}}{\text{Kg}}$$

Major technologies are PEM (run backwards) and alkaline (run backwards). More efficient] No Pt needed.

$$\text{Power} = 53.4 \rightarrow 70 \frac{\text{KW-hr}}{\text{kg}}$$

62 $\rightarrow$ 47% Efficiency.
based on H₂ avail.

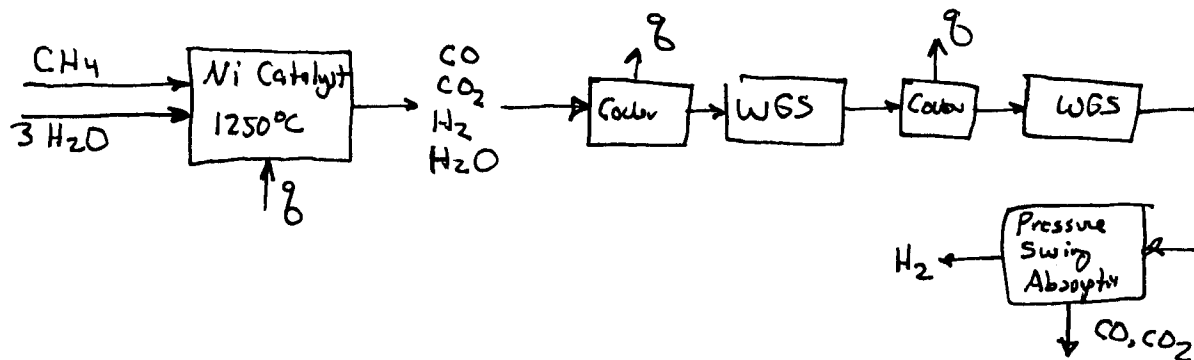
Major cost is electricity:

$$\frac{0.055 \$}{\text{KW-hr}} \times \frac{60 \text{ KW-hr}}{\text{kg}} \times \frac{\text{Kg}}{120,000 \text{ MJ}} = \frac{0.0275 \$}{\text{MJ}} \quad \left[\begin{array}{l} \text{Just wholesale elect} \\ \text{no capital, no} \\ \text{retail markup,} \\ \text{no taxes} \end{array} \right]$$

$$\text{Gasoline: } \frac{2.5 \$}{\text{gal}} \times \frac{\text{gal}}{145,000 \text{ Btu}} \times \frac{\text{Btu}}{1.054 \text{ KJ}} \times \frac{10^3 \text{ KJ}}{\text{MJ}} = 0.0163 \$/\text{MJ}$$

Won't work well unless electricity costs can be made low.

Most H₂ is via Steam Reforming: [Large central plant option].



Reformer:

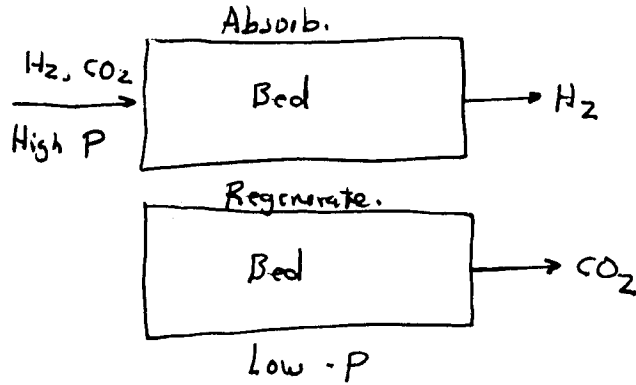
- Reaction is endothermic
- Need Heat source (CH_4)
- Outlet is equilibrium.

• Cost?



- Favoured to right at low-T
- But reaction rate is reduced by lower-T
⇒ Catalyst
⇒ Do in stages.

- Pressure Swing



Overall:

$$\eta = \frac{\text{H}_2 \text{ energy (HHV)}}{\text{CH}_4 + \text{elect} + \text{Steam}} = 69.1\%$$

- Plant generates excess steam. ⇒ If used externally ⇒ 89%

A

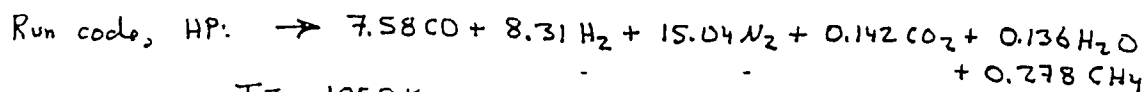
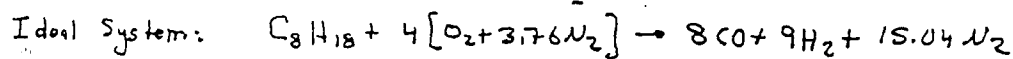
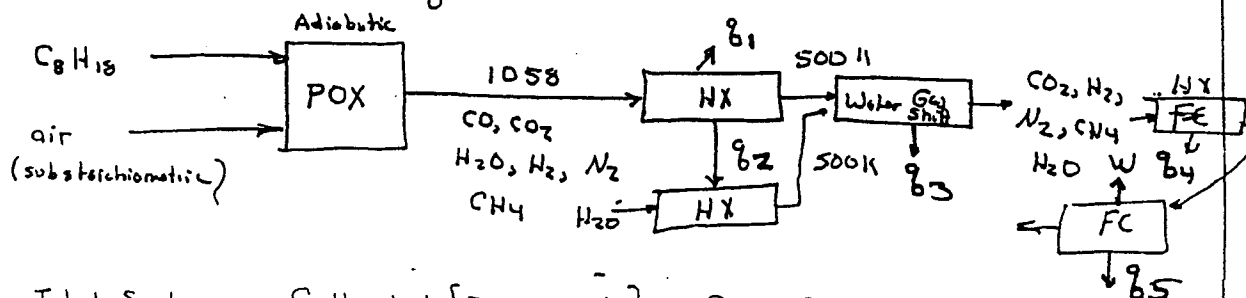
Other major approach is partial oxidation (POX).

→ Less efficient than steam, but

→ Requires much less plant.

→ Will work on liquid fuels

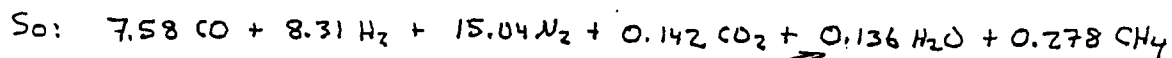
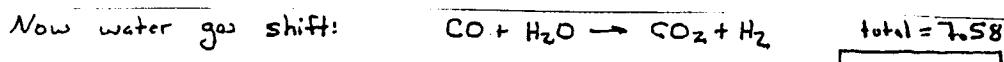
→ Choice for on-board reforming



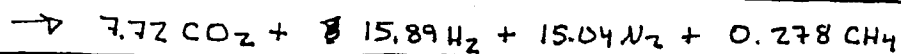
$$T = 1058 K$$

$$q_{HX}: \quad q = \Delta h = h_{1058} - h_{500}$$

$$q_1 + q_2 = 550,200 \text{ kJ/kmole } C_8H_{18}$$



add 7.444 H₂O



$$\text{Get } q_2 \text{ for } H_2O = h_{f,500} + \int_{298}^{500} C_{p,H_2O} dT = 43,961 + 6960 = 50,921 \text{ kJ/kmole } H_2O$$

$$\text{or } [7.444][50,921] = 379,100 \text{ kJ/kmole } C_8H_{18}$$

$$q_{\text{shift}} = \frac{h_P - h_R}{500K} = -302,200 \text{ kJ/kmole } C_8H_{18}$$

$$= q_3$$

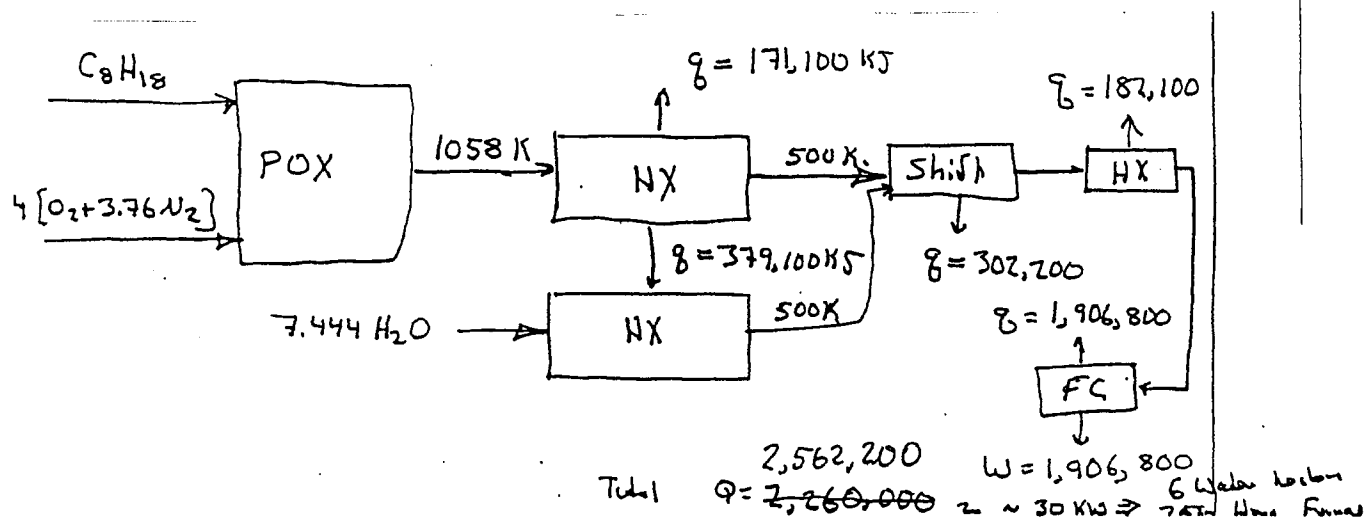
$$q_4 = h_{353} - h_{500} = -182,000$$

Dec. 5

$$\text{LHV of } \text{H}_2 = [15.87][240,000] = 3,813,600 \text{ kJ/kmole } \text{C}_8\text{H}_{18}$$

$$50\% = 1,906,800 = \dot{Q}_5 = W_{\text{elect.}}$$

So:



$$\frac{50 \text{ kW unit}}{s} \mid \frac{\text{kmole } \text{C}_8\text{H}_{18}}{1,906,800 \text{ kJ}} = 2.62 \text{ E-}5 \frac{\text{kmole}}{s} \Rightarrow 4.14 \text{ gal/hr}$$

$$\Rightarrow 67.0 \text{ kW of } \dot{Q} \Rightarrow 13 \text{ water heaters.}$$

Maybe a good deal if you need to heat, but a hard sell for mobile.

$$\text{Efficiency:} = \frac{W_{\text{elect}}}{\text{LHV of } C_8H_{18}} = \frac{1,906,800}{5,065,000} = \boxed{37.6\%}$$

Current cars: ~~well~~ Well $\rightarrow$ wheel $\sim 16\%$.

But: Optimized IC engine: [one torque, one rpm] $\rightarrow 33-37\%$
 $\Rightarrow$ Requires battery, electric motor, regen braking, etc.

Fuel cell will require the same, so no clear advantage except zero pollution.

$\Rightarrow$ Shine is off mobile?

Look at assessment and challenges for PEM.

Promises: • High potential η
 • No pollution (except CO_2 @ reformer).

Cell Design:

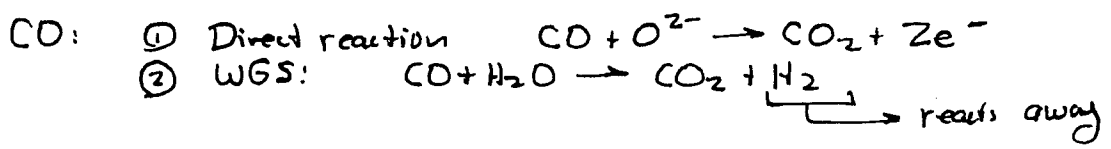
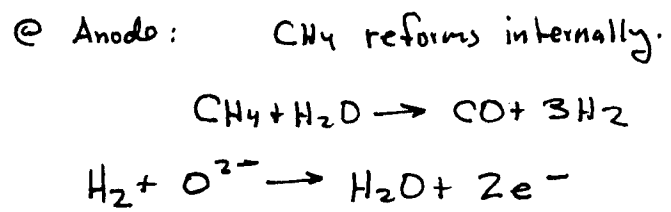
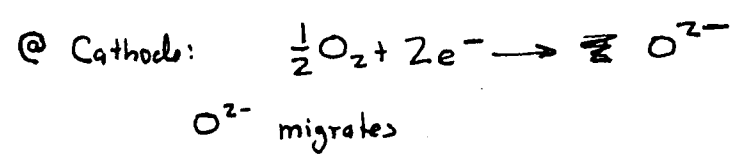
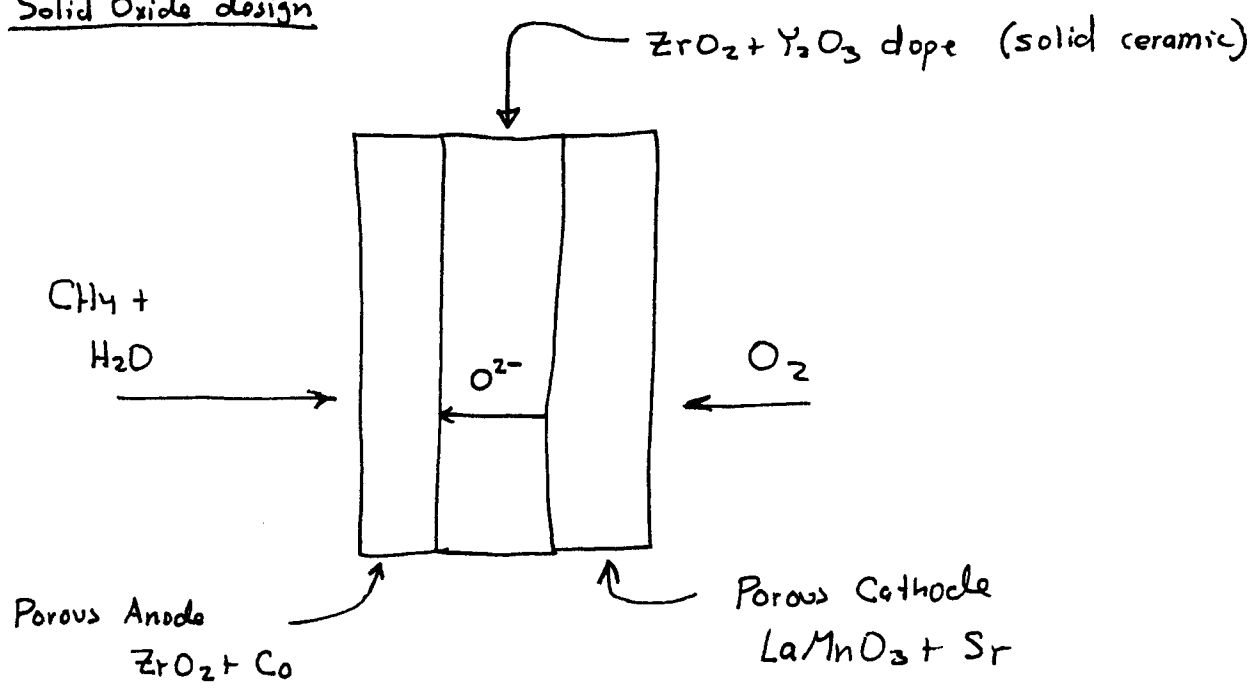
- Seeking max amp/cm² $\Rightarrow$ Pushes you towards miniaturization
 $\Rightarrow$ Microfabrication technology.
- Costs are the killer
 - Membrane too expensive
 - Electrode Pt loading too high.
 - Lower loadings are more susceptible to CO (< 2 ppm).
 - also sulfur (ppb range).
 - Distributor plate manufacturing.

Need more than economies of scale,
 need technological breakthrough.

H₂ Supply:

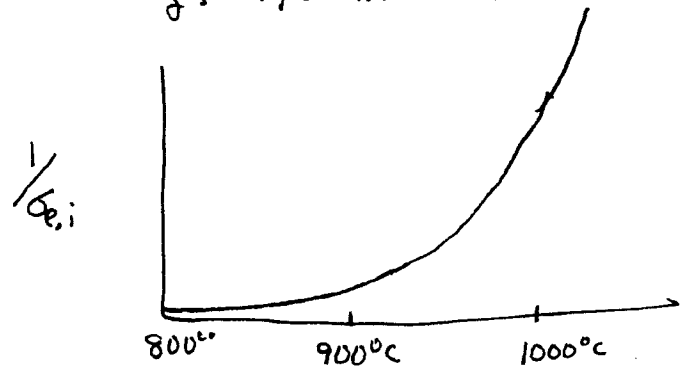
- Fossil Fuels:
 - NG $\rightarrow$ Steam reform
 - Gasoline $\rightarrow$ POX
- 50% w/o heat rec.
- Only recover a fraction of the original fuel value as H₂ LHV.
- Integrate heat rejection into bottoming cycle for stationary?
- Mobile:
 - ① Make H₂ centrally and carry on vehicle
 - $\rightarrow$ Need H₂ distribution infrastructure
 - $\rightarrow$ H₂ storage a problem
 - 5000 psi tanks
 - Cryogenic
 - Metal hydride
 - Palladium
 - Nanotubes
 - ② Carry gasoline and reform on the fly
 - $\rightarrow$ Weight
 - $\rightarrow$ Startup time (10-15 min).
 - $\rightarrow$ Large heat rejection in mobile POX that cannot be used.
- CO₂ pollution still the same.

Solid Oxide design



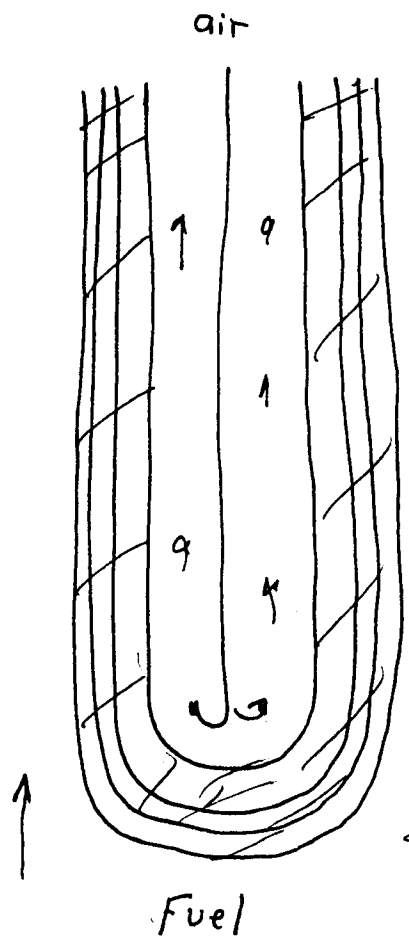
Again, even though you are hot, the steady drain of H_2 away continually shifts reaction to right.

Key point: conductivity of electrolyte do O^{2-} $[1/\sigma_{e,i}]$ is strong, exponential function of T .



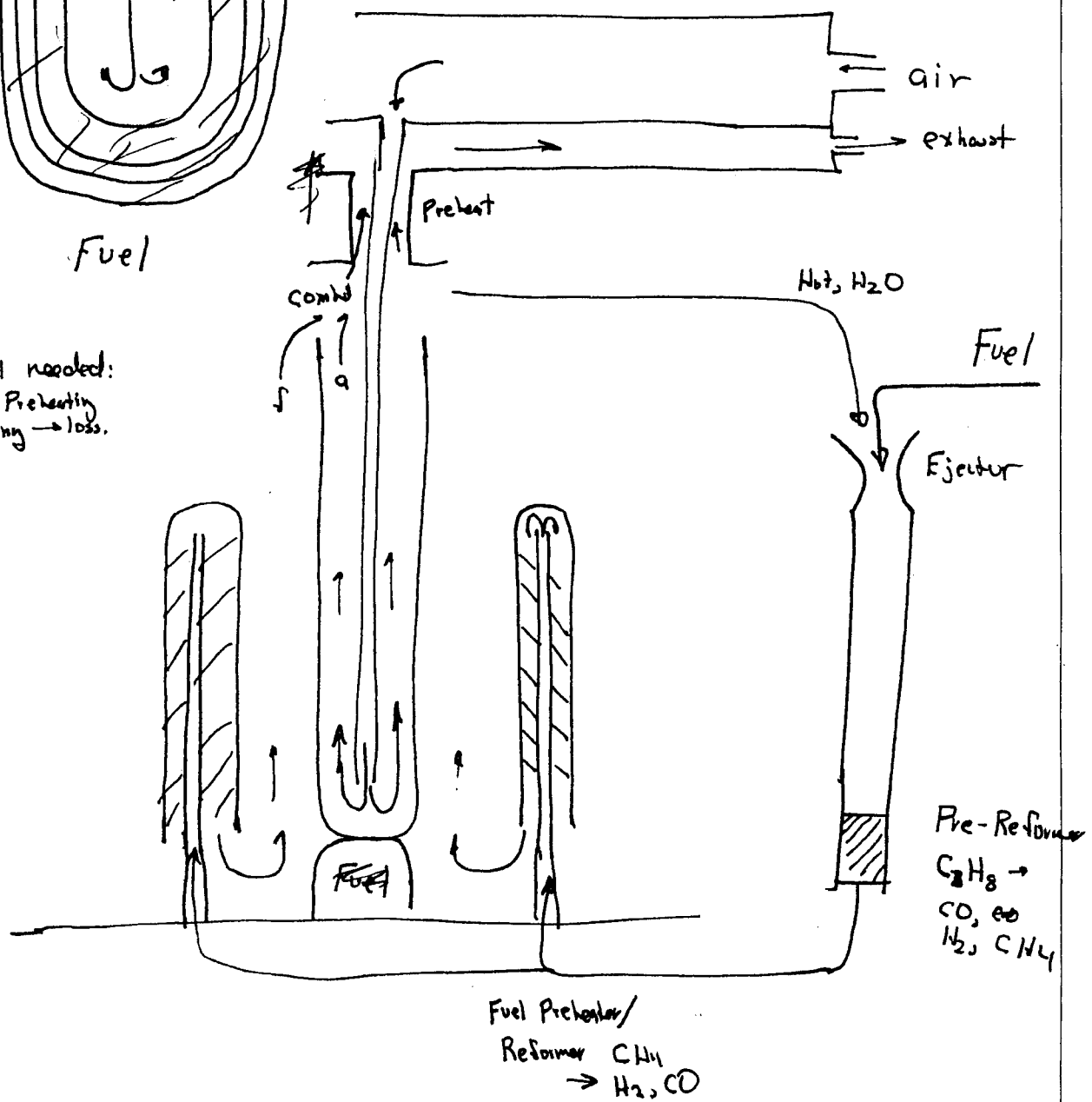
- ⇒ Must run hot!
- ⇒ All ceramic design
- ⇒ No metal.
- ⇒ Sealing a problem.

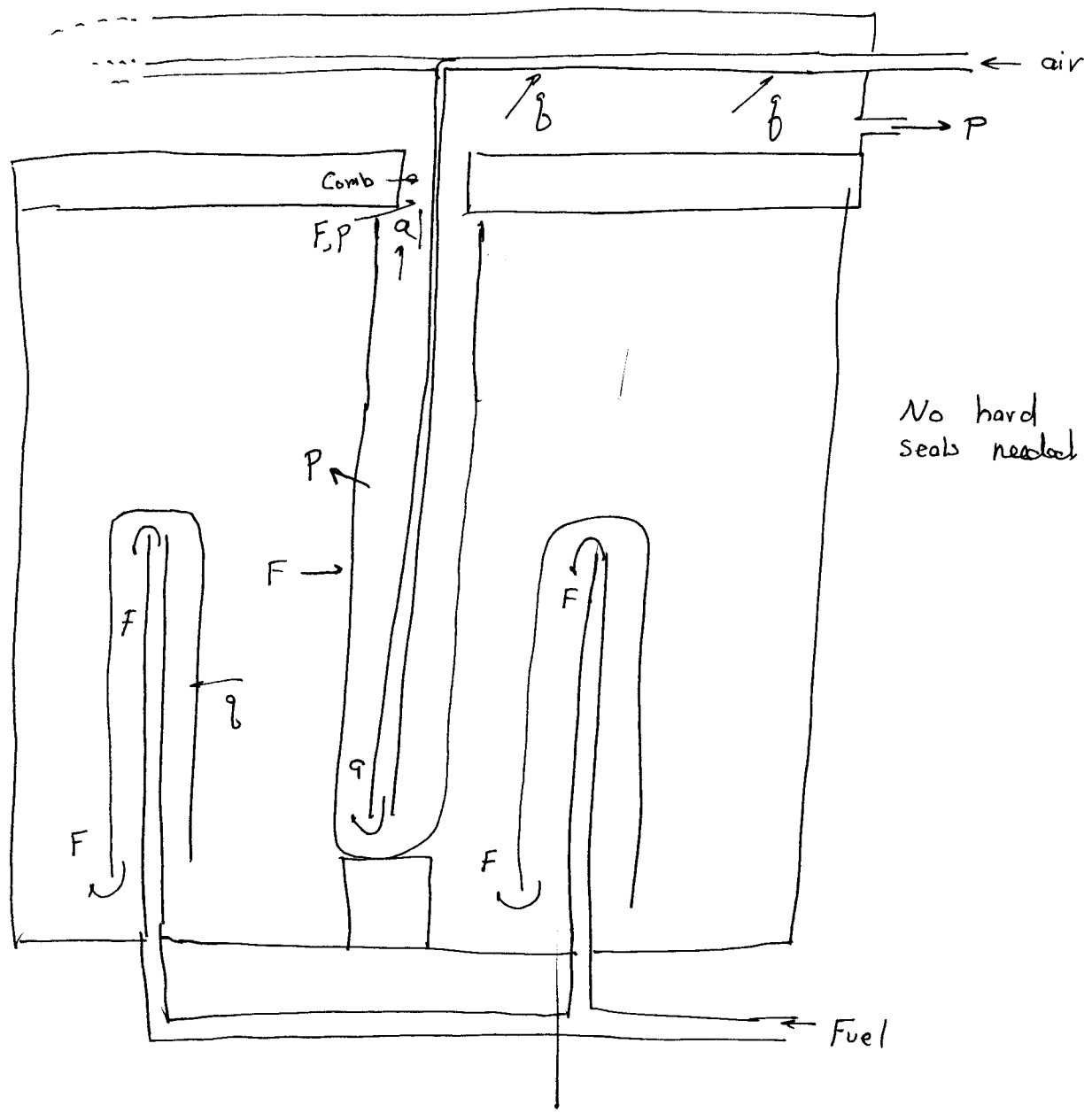
Two designs: Planar & Tubular
 ↑ Similar to PEM.



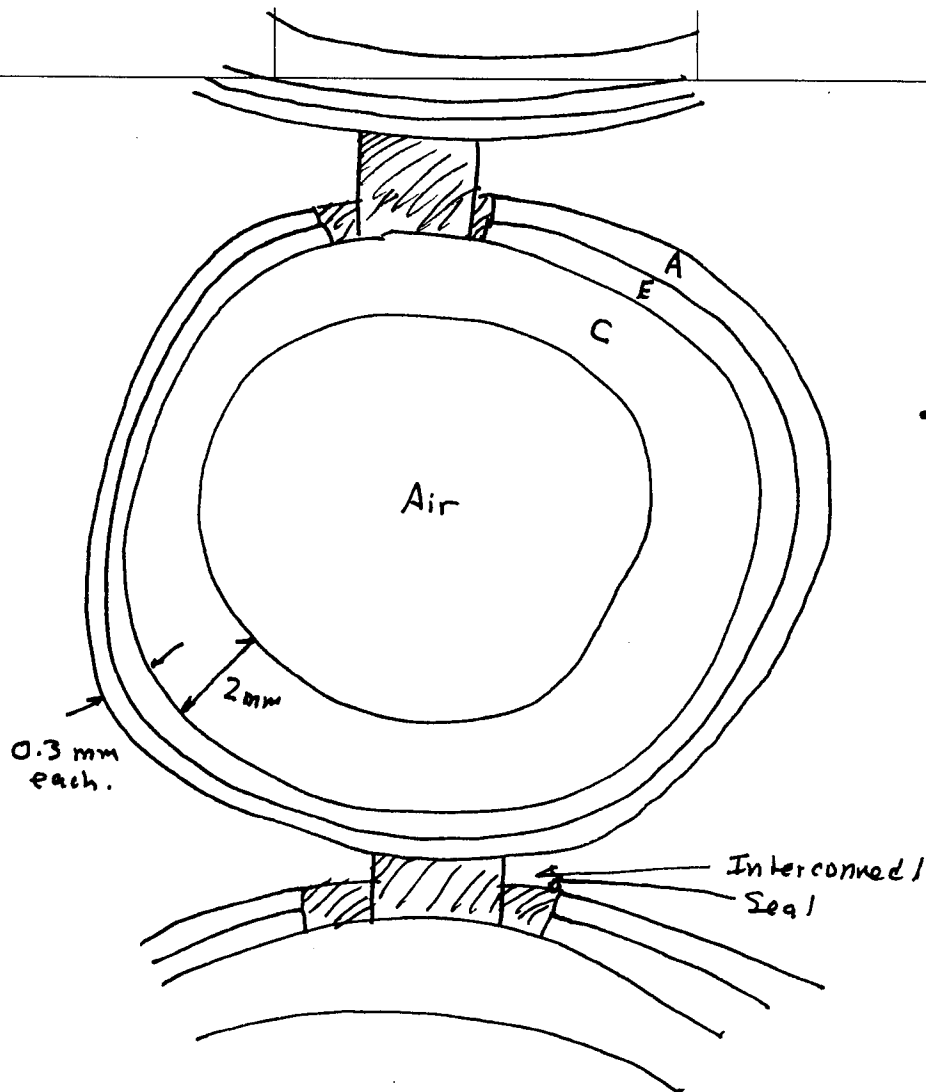
Dec 6

- No seal needed:
- Internal Preheating
- Air cooling → loss.

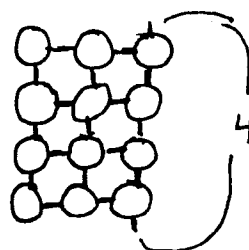




CO/
H₂



- Cast/Extrude cathode
- 1 cm across
- 2 mm thick
- Deposit electrolyte and anode (0.3 mm each).



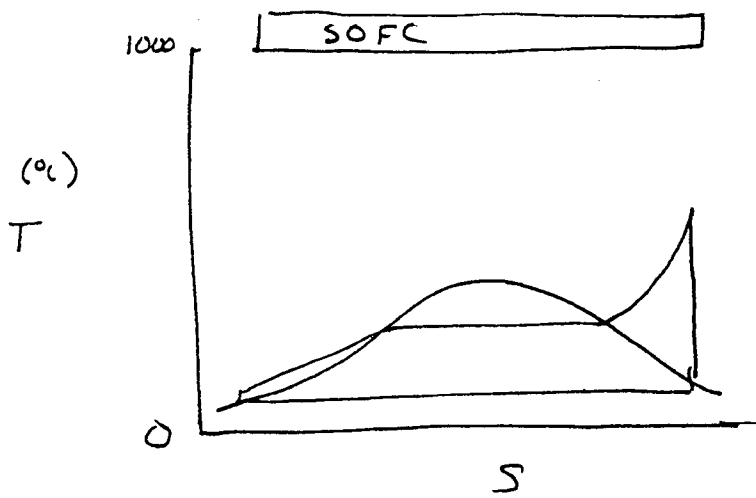
$$4V = 4 (1V)$$

- Activation overpotential low (high-T)
- Most is ohmic. (cathode, interconnect contact resistances).

Focus of cell research

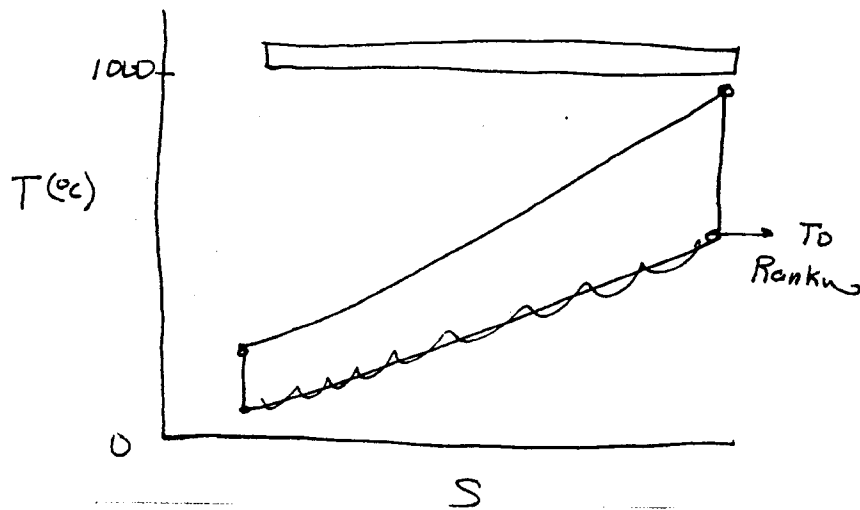
- Lower T
 - ⇒ Use common metals for materials of construction
 - ⇒ Use help with bottoming cycle integration
- Thermal stresses - must ~~match~~ either match, or design to avoid fracture.
- Bottoming cycle integration.

Here we have a problem:

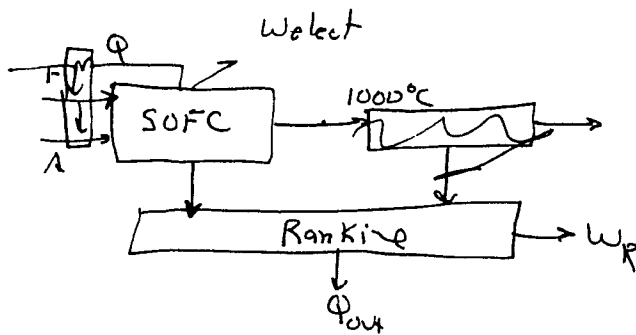


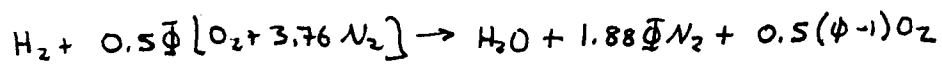
big ΔT for Q .

• Even gas turbine is tough, but better



Now have
FC + Brayton
+ Rankine.





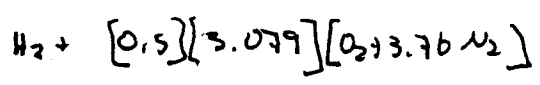
	$\frac{K_{molar}}{1}$	$\frac{h_f^\circ}{0}$	$\frac{h-h_{298}}{0}$	$\frac{n_i(h_f^\circ + h - h_{298})}{0}$	
H_2					
O_2	0.5 ϕ	0	23,513 - 8682	7415.5 ϕ	} $h_R = 39,929\phi$
N_2	1.88 ϕ	0	22,772 - 8669	26,514 ϕ	
H_2O	1	-241,820	47,500 - 9904	-204,222	} $h_P = 73,181\phi$
N_2	1.88 ϕ	0	39,000 - 8669	57,022 ϕ	
O_2	0.5($\phi-1$)	0	41,000 - 8682	16,159 ϕ - 16,159	

$-w = h_P - h_R$

$-120,000 = 73,181\phi - 222,381 - 39,929\phi$

$102,381 = 33,252\phi$

$\phi = 3.079$



$2 + [0.5][3.079][32 + 3.76(28)] = 213.343 \quad (N_2 = 2)$

$W_c = \dot{m}_a C_p (T_2 - T_1) = [213.343][1.005][410 - 300] =$

$W_c = 23,364 \text{ KJ/Kwh } H_2$

$W_T = \dot{m}_p C_p (T_4 - T_3) = [213.343][1.005][1273 - 930] = 73,543 \text{ KJ/Kwh } H_2$

$W_{net} = 120,000 + 73,543 - 23,364 = 170,179$

$\eta = \frac{170,179}{240,000} = 70.9\%$

Better $\rightarrow$ More rev sys, Woune - Losses.

Dec 8

Economics: Materials:

	$\$/m^2$	
Anode	126	} $\sim 60\%$ of stack cost -
Cathode	15	
Electrolyte	6	
Interconnect	119	

$\frac{266\$}{m^2} \mid \frac{cm^2}{0.25w} \mid \frac{m^2}{10^4 cm^2} \mid \frac{10^3 w}{KW} = 106 \$/KW$

$177 \$/KW$

- $\Rightarrow$ Increased power density critical since material cost high.
- $\Rightarrow$ Electrolyte thickness most important critical parameter [not materials, but power density]
- $\Rightarrow$ Too thin, and defect rate up.
- $\Rightarrow$ 1% defect rate $\Rightarrow$ stack cost 90 $\rightarrow$ 200 $\$/KW$.
- $\Rightarrow$ Projected large-scale mfr. cost for stack is 90-100 $\$/KW$, + Bal of plant

[Comb. Cycle = \$400-500, PEM mobile with POX reformer = \$300
 (60%) H_2 ($\sim 30\%$)
 IC engine - \$35. {Fuel Cost + η }

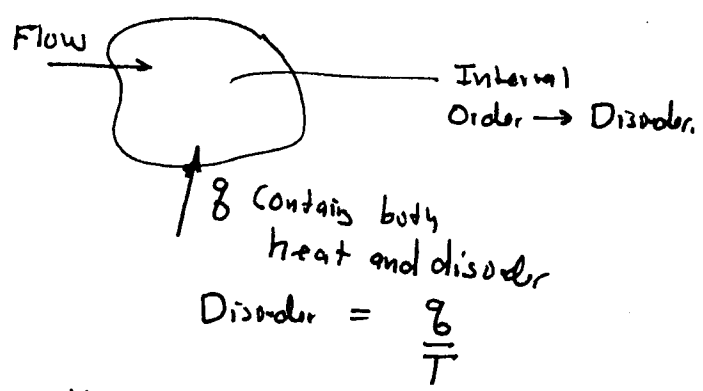
Summary:

	\$/kW	Fuel Cost (\$/10 ⁶ Btu)	η	Uncertainty
Comb. Cycle	400-500	8.	60%	Gas Cost
PEM + Mobile Ref.	300	23.	30	Fuel/Capital
IC Engine	35	23.	18	Fuel cost
SOFC / BoHm.	90 + ?	8 (CH ₄)	70	Technology
Coal - Supercritical	1200	1.5	42	Low
IGCC	1100	1.5	45	Technology
Nuclear	?	?	?	?

Two Goals

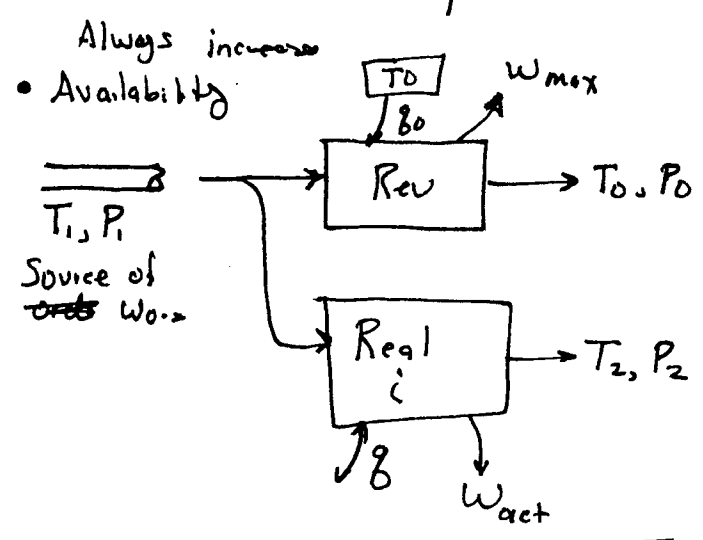
Tools: Modern Tools for performance analysis

- 1st Law.
- 2nd Law $\Rightarrow$ Energy Disorder as a property



Technologies

- Nat gas cc
 - IGCC
 - Conv. Coal Tech
 - Nuc.
 - Fuel Cell
- $\Rightarrow$ Provide a broad intro.
- $\Rightarrow$ If you work here, will need more
- $\Rightarrow$ Trend $\Rightarrow$ ~~less raw~~ more η , more capital, more brains, less raw resource
- $\Rightarrow$ Real goal in rubbing your faces in all the work was to get you down the path of thinking on our
- $\Rightarrow$ Real life has no examples.
- $\Rightarrow$ Need practice: had walk to master.



$$W_{max} = W_{act} + \sum i + \text{Avail work } Q + \text{Avail work } T_2, P_2$$

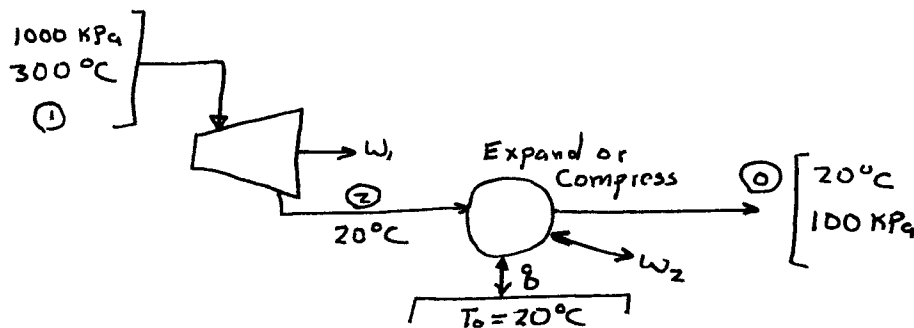
THE END?

ME 430/599C – Advanced Energy

Problem Set 1 – Assigned September 26, Due Monday, October 1, 4:30PM

1. You have steam available at 300°C and 1000 kPa. The environment is at 20°C and 100 kPa.
 - (a) Construct and present a totally reversible flow process for converting this stream to the dead state, and calculate the amount of work obtained (kJ/kg).
 - (b) Next, calculate the availability of the steam using the equation from the handout (your answer should be the same as part (a))
2. You have a flow of air at 1000 kPa, 1000 K. You have a need in your plant for air at 200 kPa, 400 K. The ambient is at 100 kPa, 300 K. Use the variable specific heat treatment.
 - (a) Construct and present a totally reversible flow process connecting these two points and calculate the amount of work obtained (kJ/kg)
 - (b) Calculate the reversible work from the equation in the handout (again, your answer should be the same as part (a))
3. The original air from problem 2 is expanded in an adiabatic, irreversible turbine to 200 kPa and 800 K.
 - (a) Find the availability of the original stream and the turbine work
 - (b) Find the irreversibility of the turbine
 - (c) Find the availability of the exhaust, and show that the sum of the irreversibility plus the work plus the availability of the exhaust equals the availability of the original inlet stream. By showing this, you have accounted for all the work potential associated with the original inlet stream.

- ① (a) The easiest approach is to use two steps: (1) adiabatic, reversible expansion to 20°C , followed by (2) isothermal expansion or compression to 100 kPa.



① 1000 kPa
 300°C $\rightarrow$ $h_1 = 3051.2 \text{ kJ/kg}$
 $S_1 = 7.1229 \text{ kJ/kg}\cdot\text{K}$

② 20°C
 $S_2 = S_1$ $\rightarrow$ Sat. mix: $X_2 = \frac{S_2 - S_f}{S_{fg}} = \frac{7.1229 - 0.2966 \text{ kJ/kg}\cdot\text{K}}{8.3706 \text{ kJ/kg}\cdot\text{K}}$

(props @ 20°C) $X_2 = 0.8155$

$h_2 = h_f + X_2 h_{fg} = 83.96 + [0.8155][2454.1] \text{ kJ/kg}$
 $\Rightarrow h_2 = 2085.30 \text{ kJ/kg}$

Sat @ $20^\circ\text{C} \rightarrow P_2 = 2.339 \text{ kPa}$, so we must compress

$w_1 = h_1 - h_2 = 3051.2 - 2085.3 \text{ kJ/kg} = 965.9 \text{ kJ/kg}$

- ③ Compressor is non-adiabatic but reversible, so $S_2 - S_0 + \frac{q}{T_0} = 0$

$q = T_0 (S_0 - S_2)$

20°C
 100 kPa

Approximate properties as those of saturated liquid @ $20^\circ\text{C} \Rightarrow h_0 = 83.96 \text{ kJ/kg}$
 $S_0 = 0.2966 \text{ kJ/kg}\cdot\text{K}$

$\Rightarrow q = [293.15 \text{ K}][0.2966 - 7.1229 \frac{\text{kJ}}{\text{kg}\cdot\text{K}}] = -2001.13 \text{ kJ/kg}$

First Law: $q - w_2 = h_0 - h_2 \Rightarrow -2001.13 - w_2 = 83.96 - 2085.30 \text{ kJ/kg}$
 $\Rightarrow w_2 = 0.21 \text{ kJ/kg}$

This calculation shows work coming out of the compression. This is because of rounding error. The w is $\ll$ than q and Δh , and is essentially zero. It is being calculated as the difference between two large nearly equal numbers.

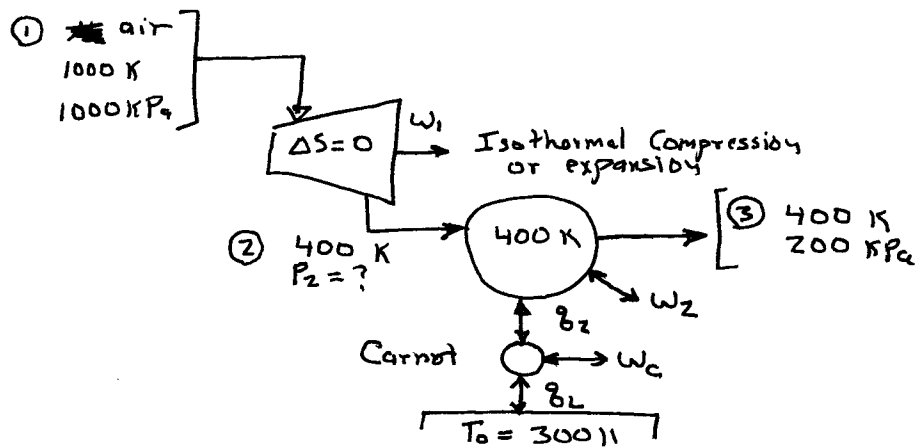
$\Rightarrow w = w_1 + w_2 = 965.9 + 0.21 \Rightarrow$

$w_{\max} = 966.11 \text{ kJ/kg}$

(b) $w_{\max} = h_1 - h_0 - T_0 (S_1 - S_0)$
 $= 3051.2 - 83.96 \text{ kJ/kg} - [293.15 \text{ K}][7.1229 - 0.2966 \frac{\text{kJ}}{\text{kg}\cdot\text{K}}]$
 $\Rightarrow w_{\max} = 966.11 \text{ kJ/kg}$

A match!

- ② There are several ways to do this problem. The example in the handout would be most closely approximated by (1) isentropic expansion to 300 K, (2) isothermal compression or expansion to same s as endstate, and (3) isentropic compression to endstate. Let's do something different



Here we do the isothermal compression or expansion @ 400 K, and use a Carnot cycle to recover the availability associated with the g .

$$\begin{aligned} \text{① } 1000 \text{ K, } 1000 \text{ kPa} &\rightarrow h_1 = 1046.04 \text{ kJ/kg} \\ &S_1^0 = 2.96770 \text{ kJ/kg-K} \\ &P_{r,1} = 114.0 \end{aligned}$$

$$\begin{aligned} \text{② } 400 \text{ K} &\rightarrow h_2 = 400.98 \text{ kJ/kg} \\ &S_2^0 = 1.99194 \text{ kJ/kg-K} \\ &P_{r,2} = 3.806 \end{aligned}$$

$$\frac{P_2}{P_1} = \frac{P_{r,2}}{P_{r,1}} \Rightarrow \frac{P_2}{1000 \text{ kPa}} = \frac{3.806}{114.0} \Rightarrow P_2 = 33.39 \text{ kPa}$$

$$w_1 = h_1 - h_2 = 1046.04 - 400.98 \text{ kJ/kg} = 645.06 \text{ kJ/kg}$$

$$\text{Entropy balance on compressor: } s_2 - s_3 + \frac{q_2}{T_2} = 0$$

$$\Rightarrow q_2 = T_2(s_3 - s_2) = (400 \text{ K})(-R \ln \frac{P_3}{P_2}) = (400 \text{ K})(-0.287 \frac{\text{kJ}}{\text{kg-K}}) \ln \left(\frac{200 \text{ kPa}}{33.39 \text{ kPa}} \right)$$

$$\Rightarrow q_2 = -205.50 \text{ kJ/kg} \quad \text{Heat out}$$

$$\text{First Law: } q_2 - w_2 = h_3 - h_2 \Rightarrow w_2 = -205.50 \text{ kJ/kg} \quad \text{Work in}$$

$$\text{We can get } w_c \text{ from Carnot efficiency: } w_c = q_2 \left[1 - \frac{T_L}{T_H} \right] = (+205.50 \frac{\text{kJ}}{\text{kg}}) \left[1 - \frac{300}{400} \right]$$

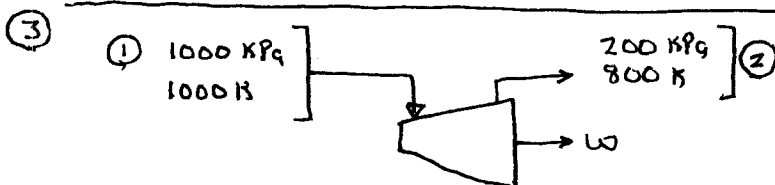
$$\Rightarrow w_c = +51.38 \frac{\text{kJ}}{\text{kg}} \quad \text{Work out}$$

$$\Rightarrow w_{\max} = w_1 + w_2 + w_c = 645.06 + (-205.50) + (+51.38) \frac{\text{kJ}}{\text{kg}}$$

$$\Rightarrow w_{\max} = 490.94 \text{ kJ/kg}$$

$$\begin{aligned} \text{(b) } w_{\max} &= h_1 - h_3 - T_0(S_1 - S_3) \\ &= h_1 - h_3 - T_0(S_1^0 - S_3^0 - R \ln \frac{P_1}{P_3}) \\ &= 1046.04 - 400.98 \frac{\text{kJ}}{\text{kg}} - (300 \text{ K}) \left[2.9677 - 1.99194 \frac{\text{kJ}}{\text{kg-K}} - (0.287 \frac{\text{kJ}}{\text{kg-K}}) \ln \left(\frac{1000}{200} \right) \right] \\ &\Rightarrow w_{\max} = 490.91 \text{ kJ/kg} \end{aligned}$$

Matches 8



$$\textcircled{1} \left. \begin{array}{l} 1000 \text{ kPa} \\ 1000 \text{ K} \end{array} \right\} \rightarrow \begin{array}{l} h_1 = 1046.04 \text{ kJ/kg} \\ s_1^0 = 2.9677 \text{ kJ/kg} \cdot \text{K} \\ P_{r,1} = 114.0 \end{array}$$

$$\textcircled{2} \left. \begin{array}{l} 200 \text{ kPa} \\ 800 \text{ K} \end{array} \right\} \rightarrow \begin{array}{l} h_2 = 821.95 \text{ kJ/kg} \\ s_2^0 = 2.71787 \text{ kJ/kg} \cdot \text{K} \\ P_{r,2} = 47.75 \end{array}$$

$$\textcircled{3} \left. \begin{array}{l} 300 \text{ K} \\ 100 \text{ kPa} \end{array} \right\} \rightarrow \begin{array}{l} h_0 = 300.19 \text{ kJ/kg} \\ s_0^0 = 1.70203 \text{ kJ/kg} \cdot \text{K} \\ P_{r,0} = 1.386 \end{array}$$

10 Points

$$(a) W_{\max} = h_1 - h_0 - T_0 (s_1 - s_0) = 1046.04 - 300.19 \frac{\text{kJ}}{\text{kg}} - (300 \text{ K}) \left[2.9677 - \frac{1.70203}{\text{K}} - (0.287 \frac{\text{kJ}}{\text{kg} \cdot \text{K}}) \ln \frac{1000}{100} \right]$$

$$\Rightarrow W_{\max} = 564.40 \frac{\text{kJ}}{\text{kg}}$$

$$W_T = h_1 - h_2 = 1046.04 - 821.95 \frac{\text{kJ}}{\text{kg}} \Rightarrow W_T = 224.09 \frac{\text{kJ}}{\text{kg}}$$

$$(b) i_T = T_0 (s_2 - s_1) = T_0 (s_2^0 - s_1^0 - R \ln \frac{P_2}{P_1})$$

$$= (300 \text{ K}) \left[2.71787 - 2.9677 \frac{\text{kJ}}{\text{kg} \cdot \text{K}} - (0.287 \frac{\text{kJ}}{\text{kg} \cdot \text{K}}) \ln \frac{200}{1000} \right] \Rightarrow i_T = 63.62 \frac{\text{kJ}}{\text{kg}}$$

$$(c) W_{\max, \text{exhaust}} = h_2 - h_0 - T_0 (s_2 - s_0) = h_2 - h_0 - T_0 (s_2^0 - s_0^0 - R \ln \frac{P_2}{P_0})$$

$$= 821.95 - 300.19 \frac{\text{kJ}}{\text{kg}} - (300 \text{ K}) \left(2.71787 - 1.70203 \frac{\text{kJ}}{\text{kg} \cdot \text{K}} - (0.287 \frac{\text{kJ}}{\text{kg} \cdot \text{K}}) \ln \frac{200}{100} \right)$$

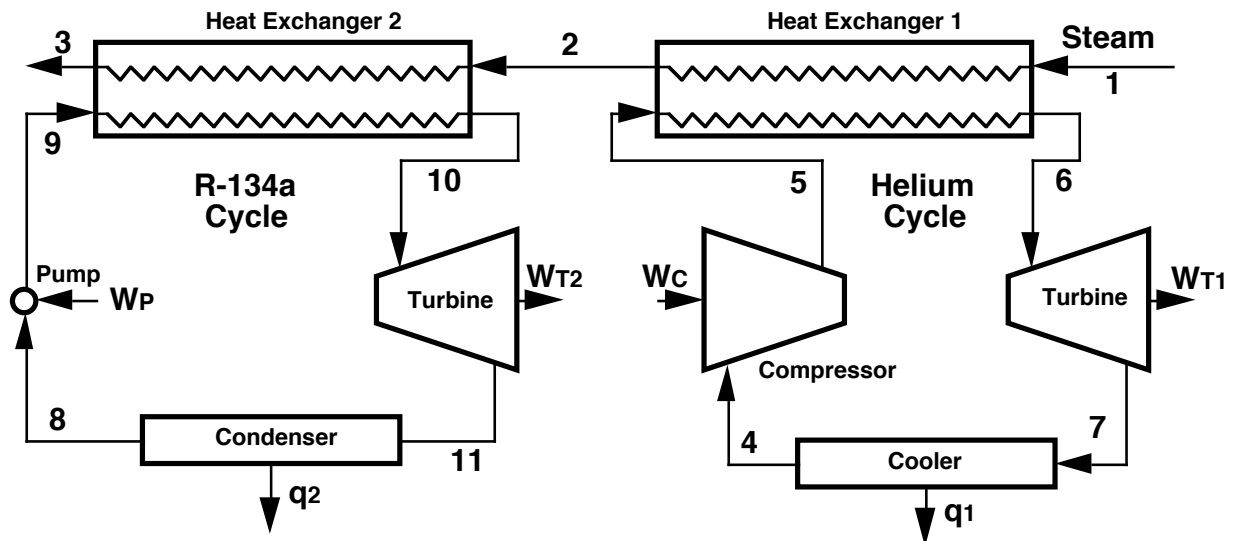
$$\Rightarrow W_{\max, \text{exhaust}} = 276.69 \frac{\text{kJ}}{\text{kg}}$$

	$\frac{\text{kJ}}{\text{kg}}$	%
Original Availability	564.40	100
Turbine Work	224.09	39.70
Turbine irreversibility	63.62	11.27
Lost with exhaust	276.69	49.03
Σ	564.40	Match 0

Biggest loss is with exhaust, not i_T

ME 430/599C – Advanced Energy
Problem Set 2 – Assigned October 2, Due Monday, October 8, 4:30PM

Steam is available from geothermal beds at atmospheric pressure and relatively high temperatures. It is generally fairly dirty and is not used directly in cycles, but instead is used as a heat source for indirectly heated cycles. The steam gives up sensible heat as it cools to around 100°C , and then gives up latent heat as it condenses. The most reversible systems may use two cycles to absorb the heat, one that matches the cooling that occurs during the sensible heat extraction, and a second cycle that isothermally absorbs the latent heat released by condensation. One such system is shown here:



A closed helium gas turbine cycle is used to extract much of the sensible heat, while an R-134a cycle is used to extract the remainder of the sensible heat and the latent heat. The properties of these cycles are as follows:

Steam: The steam available to the cycle from the geothermal bed is at 800°C , 100 kPa. This is cooled to 350°C by the helium heat exchanger. The R-134a heat exchanger further cools the steam and condenses it to a saturated liquid at 100 kPa, which is exhausted.

Helium Cycle: The low pressure and high pressure parts of the cycle are 1 and 4 atm, respectively. The helium is heated to 1000 K at the outlet of the heat exchanger. The turbine is adiabatic with an efficiency of 87%. The cooler reduces the outlet temperature of the turbine to 310 K by transferring heat to the environment, which is at 20°C , 100 kPa. The compressor is adiabatic with an efficiency of 85%.

R-134a Cycle: The low pressure and high pressure parts of the cycle are at 0.8 and 3.0 MPa, respectively. The outlet of the R-134a heater is a saturated vapor, and the turbine is adiabatic with an efficiency of 80%. The condenser cools the vapor to a saturated liquid. The pump can be approximated as reversible and adiabatic.

1. Find the availability of the original steam (kJ/kg).

2. Prepare a table showing all the properties, at each point in the system (T, P, h, s, X where appropriate for steam, R-134a; T, P for helium).
3. Find the ratio of the mass of helium/mass of steam, and the ratio of mass of R-134a/mass of steam.
4. Prepare a table, arranged from largest to smallest value, of the net system work, the availability of exiting streams, and the irreversibilities of each component (kJ/kg of **steam** and percent of original availability). Demonstrate that the table sums to the original availability of the steam. Note that this part of the problem should be worked on the basis of 1 kg of steam.

$$\textcircled{1} \quad \textcircled{1} \quad \left. \begin{array}{l} 800^\circ\text{C} \\ 100 \text{ kPa} \end{array} \right\} \rightarrow \begin{array}{l} h_1 = 4158.6 \text{ kJ/kg} \\ s_1 = 9.5652 \text{ kJ/kg-K} \end{array} \quad \textcircled{2} \quad \left. \begin{array}{l} 20^\circ\text{C} \\ 100 \text{ kPa} \end{array} \right\} \xrightarrow{\text{Treat as sat. liq}} \Rightarrow \begin{array}{l} h_o = 83.96 \text{ kJ/kg} \\ s_o = 0.2966 \text{ kJ/kg-K} \end{array}$$

$$W_{\max} = h_1 - h_o - T_o (s_1 - s_o) = 4158.6 - 83.96 - (293 \text{ K})(9.5652 - 0.2966) \frac{\text{kJ}}{\text{kg-K}}$$

$$\Rightarrow W_{\max} = 1358.94 \text{ kJ/kg steam}$$

② Steam:

$$\textcircled{2} \quad \left. \begin{array}{l} 350^\circ\text{C} \\ 100 \text{ kPa} \end{array} \right\} \rightarrow \begin{array}{l} h_2 = 3176.25 \text{ kJ/kg} \\ s_2 = 8.3797 \text{ kJ/kg-K} \end{array}$$

$$\textcircled{3} \quad \left. \begin{array}{l} 100 \text{ kPa} \\ \text{Sat. Liq.} \end{array} \right\} \rightarrow \begin{array}{l} h_3 = 419.04 \text{ kJ/kg} \\ s_3 = 1.3069 \text{ kJ/kg-K} \end{array}$$

Helium:

$$\textcircled{4} \quad \text{Given } T_4 = 310 \text{ K}, P_4 = 1 \text{ atm.}$$

$$\textcircled{5} \quad \text{Isentropic compression: } \frac{T_5}{T_4} = \left[\frac{P_5}{P_4} \right]^{k-1/k} \Rightarrow \frac{T_5}{310} = \left[\frac{4}{1} \right]^{\frac{0.667}{1.667}}$$

$$\Rightarrow T_{5,s} = 539.83 \text{ K}$$

$$\eta_c = \frac{W_s}{W_a} = \frac{h_{5,s} - h_4}{h_5 - h_4} = \frac{C_p (T_{5,s} - T_4)}{C_p (T_5 - T_4)} \Rightarrow 0.85 = \frac{539.83 - 310}{T_5 - 310}$$

$$\Rightarrow T_5 = 580.4 \text{ K}$$

$$\textcircled{6} \quad T_6 = 1000 \text{ K}, P_6 = 4 \text{ atm}$$

$$\textcircled{7} \quad \text{Isentropic expansion } \frac{T_7}{T_6} = \left[\frac{P_7}{P_6} \right]^{k-1/k} \Rightarrow \frac{T_7}{1000} = \left[\frac{1}{4} \right]^{\frac{0.667}{1.667}}$$

$$\Rightarrow T_{7,s} = 574.25 \text{ K}$$

$$\eta_T = \frac{W_a}{W_s} = \frac{h_6 - h_7}{h_6 - h_{7,s}} = \frac{C_p (T_6 - T_7)}{C_p (T_6 - T_{7,s})} \Rightarrow 0.87 = \frac{1000 - T_7}{1000 - 574.25}$$

$$\Rightarrow T_7 = 629.6 \text{ K}$$

R-134a:

$$\textcircled{8} \quad \left. \begin{array}{l} 0.8 \text{ MPa} \\ \text{Sat. Liq.} \end{array} \right\} \rightarrow \begin{array}{l} h_8 = 93.42 \text{ kJ/kg} \\ s_8 = 0.3459 \text{ kJ/kg-K} \end{array} \quad \begin{array}{l} v_8 = 0.8454 \text{ E-3 m}^3/\text{kg} \\ T_8 = 31.33^\circ\text{C} \end{array}$$

$$\textcircled{9} \quad \text{Isentropic Pump } W_p = v_8 (P_9 - P_8) = (0.8454 \text{ E-3 m}^3/\text{kg})(3000 - 800 \text{ kPa})$$

$$\Rightarrow W_p = 1.86 \text{ kJ/kg}$$

$$h_9 = h_8 + W_p = 93.42 + 1.86 \text{ kJ/kg} \Rightarrow h_9 = 95.28 \text{ kJ/kg}$$

$$\textcircled{10} \quad \left. \begin{array}{l} 3 \text{ MPa} \\ \text{Sat. Vap.} \end{array} \right\} \rightarrow \begin{array}{l} h_{10} = 278.01 \text{ kJ/kg} \\ s_{10} = 0.8735 \text{ kJ/kg-K} \end{array} \quad \begin{array}{l} T_{10} = 86.22^\circ\text{C} \end{array}$$

$$\textcircled{11} \quad \text{Isentropic: } \left. \begin{array}{l} 0.8 \text{ MPa} \\ s_{11} = s_{10} \end{array} \right\} \rightarrow \begin{array}{l} \text{Sat mix} \\ x_{11,s} = \frac{s_{11,s} - s_f}{s_{fg}} = \frac{0.8735 - 0.3459 \text{ kJ/kg-K}}{0.9066 - 0.3459 \text{ kJ/kg-K}} = 0.9410 \end{array}$$

$$h_{11,s} = h_f + x_{11,s} h_{fg} = 93.42 + [0.9410][170.73] \frac{\text{kJ}}{\text{kg}} = 254.07 \frac{\text{kJ}}{\text{kg}}$$

$$\eta_T = \frac{W_a}{W_s} = \frac{h_{10} - h_{11}}{h_{10} - h_{11,s}} \Rightarrow 0.8 = \frac{278.01 - h_{11}}{278.01 - 254.07} \Rightarrow h_{11} = 258.86 \frac{\text{kJ}}{\text{kg}}$$

$$\text{Now real } x_{11} = \frac{h_{11} - h_f}{h_{fg}} = \frac{258.86 - 93.42 \text{ kJ/kg}}{170.73} = 0.9690$$

$$\text{Finally, real } s_{11} = s_f + x_{11} s_{fg} = 0.3459 + [0.9690][0.9066 - 0.3459] \frac{\text{kJ}}{\text{kg-K}}$$

$$\Rightarrow s_{11} = 0.8892 \text{ kJ/kg-K.}$$

Table follows:

Property Summary

State	Temperature		Pressure	h	s	x
	K	°C	kPa	kJ/kg	kJ/kg-K	
1	1073	800	100	4158.6	9.5652	
2	623	350	100	3176.25	8.3797	
3	373	100	100	419.04	1.3069	0
4	310	37	101			
5	580.4	307.4	404			
6	1000	727	404			
7	629.6	356.6	101			
8	304.33	31.33	800	93.42	0.3459	
9	304.33	31.33	3000	95.28	0.3459	
10	359.22	86.22	3000	278.01	0.8735	
11	304.33	31.33	800	258.86	0.8892	0.969
Dead Steam	293	20	100	83.96	0.2966	Comp Liq

③ Helium: 1st Law on HX

$$\begin{aligned}
 m_{st}(h_1 - h_2) &= m_{He} C_p (T_6 - T_5) \Rightarrow (1 \text{ kg}) [4158.6 - 3176.25 \frac{\text{kJ}}{\text{kg}}] \\
 &= m_{He} [5.1926 \frac{\text{kJ}}{\text{kg-K}}] [1000 - 580.4 \text{ K}] \\
 &\Rightarrow m_{He} = 0.4509 \frac{\text{kg He}}{\text{kg st}}
 \end{aligned}$$

R-134a: 1st Law on HX $m_{st}(h_2 - h_3) = m_R(h_{10} - h_9)$

$$\begin{aligned}
 \Rightarrow (1 \text{ kg}) (3176.25 - 419.04 \frac{\text{kJ}}{\text{kg}}) &= m_R (278.01 - 95.28 \frac{\text{kJ}}{\text{kg}}) \\
 \Rightarrow m_R &= 15.09 \frac{\text{kg R}}{\text{kg st}}
 \end{aligned}$$

④ Steam: Lost work at ③

$$\begin{aligned}
 W_{\max, 3} &= h_3 - h_0 - T_0 (s_3 - s_0) = 419.04 - 83.96 - (293 \text{ K}) (1.3069 - 0.2966 \frac{\text{kJ}}{\text{kg-K}}) \\
 \text{Lost Work @ 3} &= 39.06 \frac{\text{kJ}}{\text{kg st}}
 \end{aligned}$$

Helium: HX 1: $i = T_0 [m_{st}(s_2 - s_1) + m_{He}(s_6 - s_5)]$

$$\begin{aligned}
 &= T_0 [m_{st}(s_2 - s_1) + m_{He} (C_p \ln \frac{T_6}{T_5} - R \ln \frac{P_6}{P_5})] \\
 &= (293 \text{ K}) [(1 \text{ kg st}) (8.3797 \frac{\text{kJ}}{\text{kg-K}} - 9.5652 \frac{\text{kJ}}{\text{kg-K}}) + (0.4509 \text{ kg He}) (5.1926 \frac{\text{kJ}}{\text{kg-K}}) \ln \left(\frac{1000}{580.4} \right)] \\
 i_{HX1} &= 25.87 \frac{\text{kJ}}{\text{kg st}}
 \end{aligned}$$

Turbine: $i = m_{He} T_0 (s_7 - s_6) = m_{He} T_0 [C_p \ln \frac{T_7}{T_6} - R \ln \frac{P_7}{P_6}]$

$$\begin{aligned}
 &= [0.4509 \frac{\text{kg He}}{\text{kg st}}] (293 \text{ K}) [(5.1926 \frac{\text{kJ}}{\text{kg-K}}) \ln \left(\frac{629.6}{1000} \right) - (2.0769 \frac{\text{kJ}}{\text{kg-K}}) \ln \left(\frac{1}{4} \right)] \\
 \Rightarrow i_{T1} &= 62.98 \frac{\text{kJ}}{\text{kg st}}
 \end{aligned}$$

Cooler: $q = C_p (T_7 - T_4) = (5.1926 \frac{\text{kJ}}{\text{kg} \cdot \text{K}})(629.6 - 310 \text{ K}) = 1659.6 \frac{\text{kJ}}{\text{kg He}}$

$$i = m_{\text{He}} T_0 \left[S_4 - S_7 + \frac{q_R}{T_R} \right] = (0.4509 \frac{\text{kg He}}{\text{s}})(293 \text{ K}) \left[(5.1926 \frac{\text{kJ}}{\text{kg} \cdot \text{K}}) \ln \left(\frac{310 \text{ K}}{629.6} \right) + \frac{1659.6 \text{ kJ/kg He}}{293 \text{ K}} \right]$$

$$\Rightarrow i_{\text{cooler}} = 262.26 \text{ kJ/kg s}$$

Compressor: $i = m_{\text{He}} T_0 (S_5 - S_4) = m_{\text{He}} T_0 \left[C_p \ln \frac{T_5}{T_4} - R \ln \frac{P_5}{P_4} \right]$

$$= (0.4509 \frac{\text{kg He}}{\text{s}})(293 \text{ K}) \left[(5.1926 \frac{\text{kJ}}{\text{kg} \cdot \text{K}}) \ln \left(\frac{580.4}{310} \right) - (2.0769 \frac{\text{kJ}}{\text{kg} \cdot \text{K}}) \ln(4) \right]$$

$$\Rightarrow i_{\text{comp}} = 49.85 \text{ kJ/kg s}$$

$$W_T = m_{\text{He}} C_p (T_6 - T_7) = (0.4509 \frac{\text{kg He}}{\text{s}})(5.0926 \frac{\text{kJ}}{\text{kg} \cdot \text{K}})(1000 - 629.6 \text{ K})$$

$$W_{T1} = 850.53 \text{ kJ/kg s}$$

$$W_C = m_{\text{He}} C_p (T_5 - T_4) = (0.4509 \frac{\text{kg He}}{\text{s}})(5.0926 \frac{\text{kJ}}{\text{kg} \cdot \text{K}})(580.4 - 310 \text{ K})$$

$$W_C = 620.91 \text{ kJ/kg s}$$

$$\text{Net work} = W_{T1} - W_C = 850.53 - 620.91 \text{ kJ/kg s}$$

$$\Rightarrow W_{\text{net, He}} = 229.62 \text{ kJ/kg s}$$

R-134a:

HX2: $i = T_0 [m_{\text{St}} (S_3 - S_2) + m_R (S_{10} - S_9)]$

$$= (293 \text{ K}) \left[(1 \text{ kg}) (1.3069 - 8.3797 \frac{\text{kJ}}{\text{kg} \cdot \text{K}}) + (15.09 \text{ kg R}) (0.8735 - 0.3459 \frac{\text{kJ}}{\text{kg} \cdot \text{K}}) \right]$$

$$\Rightarrow i_{\text{HX2}} = 260.38 \text{ kJ/kg s}$$

R-Turbine: $i = m_R T_0 (S_{11} - S_{10}) = (15.09 \frac{\text{kg R}}{\text{s}})(293 \text{ K}) (0.8892 - 0.8735 \frac{\text{kJ}}{\text{kg} \cdot \text{K}})$

$$\Rightarrow i_T = 69.42 \text{ kJ/kg s}$$

Condenser: $q = h_{11} - h_8 = 258.86 - 93.42 \text{ kJ/kg} = 165.44 \text{ kJ/kg}$

$$i = m_R T_0 \left[S_8 - S_{11} + \frac{q_R}{T_R} \right] = (15.09 \frac{\text{kg R}}{\text{s}})(293 \text{ K}) \left[0.3459 - 0.8892 \frac{\text{kJ}}{\text{kg} \cdot \text{K}} + \frac{165.44 \text{ kJ/kg}}{293 \text{ K}} \right]$$

$$\Rightarrow i_{\text{cond}} = 94.36 \text{ kJ/kg s}$$

$$W_{T2} = m_R (h_{10} - h_{11}) = (15.09 \frac{\text{kg R}}{\text{s}})(278.01 - 258.86 \text{ kJ/kg})$$

$$W_{T2} = 288.97 \text{ kJ/kg s}$$

$$W_{\text{net}} = W_{T2} - W_P = 288.97 - \left[1.86 \frac{\text{kJ}}{\text{kg R}} \right] (15.09 \frac{\text{kg R}}{\text{s}})$$

$$W_{R, \text{net}} = 260.91 \text{ kJ/kg s}$$

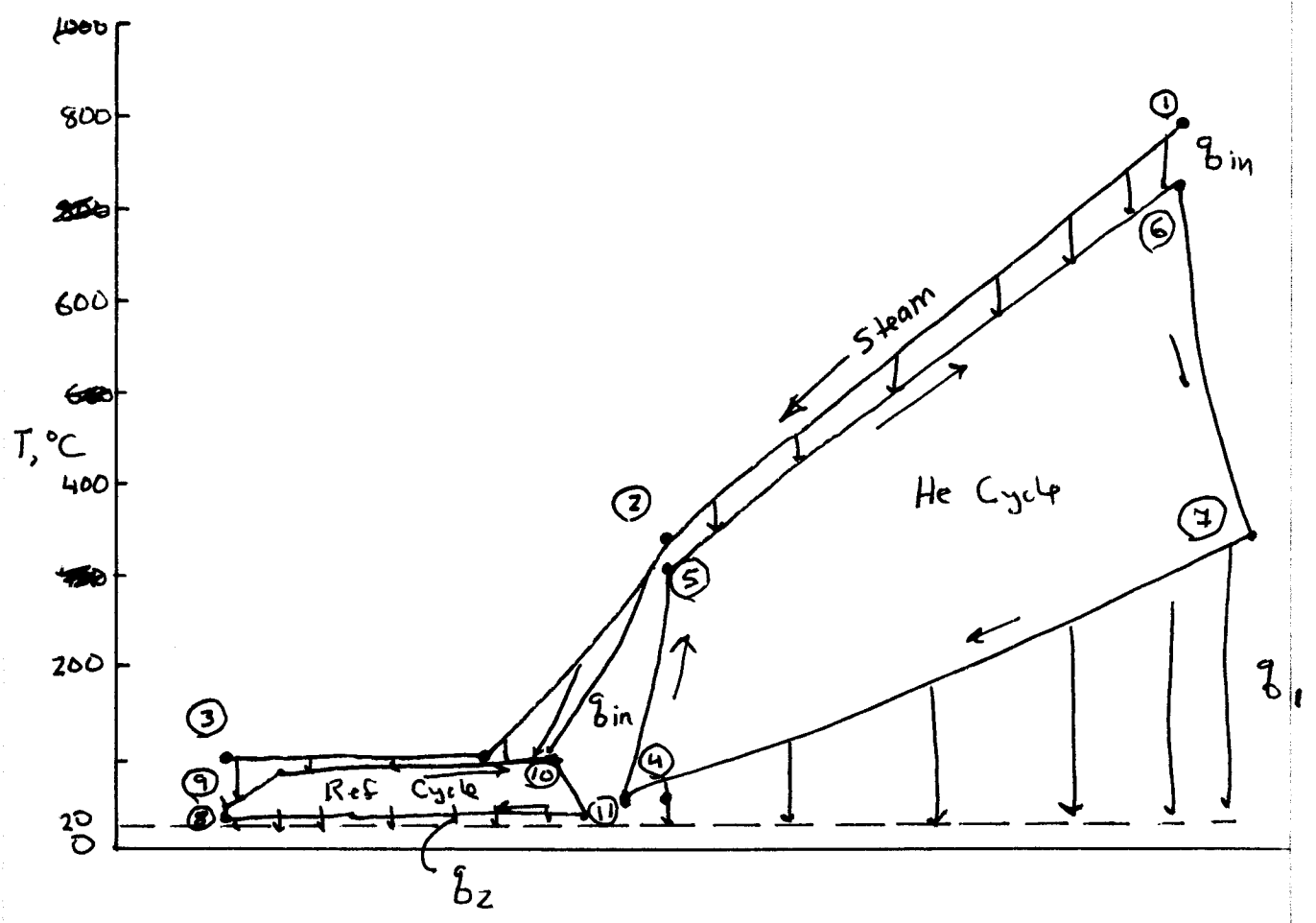
$$\text{Net system work} = W_{\text{net, He}} + W_{\text{net, R}} = 229.62 + 260.91 \text{ kJ/kg s}$$

$$W_{\text{net}} = 490.53 \text{ kJ/kg s}$$

Summary Table.

	kJ/kg steam	Percent
Original Availability	1358.94	
Net Work	490.53	36.21
Helium Cooler	262.26	19.36
Ref HX	260.38	19.22
Ref Condenser	94.36	6.97
Ref Turbine	69.42	5.12
Helium Turbine	62.98	4.65
Helium Compressor	49.85	3.68
Lost Work at 3	39.06	2.88
Helium HX	25.87	1.91
Sum	1354.71	100

T-s Diagram - See discussion on following page.



Discussion

Our availability was within 0.31% of the sum of the net work, the availability lost with exit streams, and the internal irreversibilities. Normally I get a little closer (typically 0.03%) on this type of problem. It could be due to a slight inconsistency in the tables, although I cannot rule out a small error at some point.

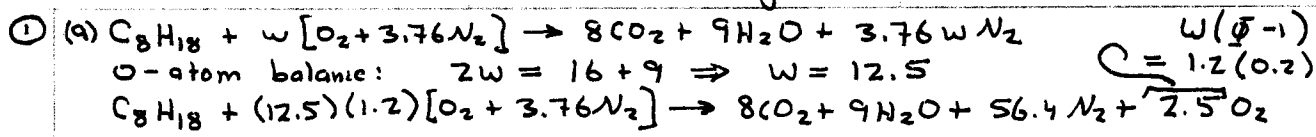
We clearly do not have a very good system since we are recovering only 36% of the work potential of the inlet steam. The two biggest problems are the helium cooler and the refrigerant heat exchanger. The easiest way to see the problem is a T-s diagram drawn to scale (shown in the solution). We see that the high helium turbine exhaust temperature has a high availability that is wasted by rejecting the heat to the environment. Some kind of bottoming cycle could be used to recover some of this work. The problem with the refrigerant heat exchanger is the high temperature of the steam at the inlet relative to that of the refrigerant being boiled.

The irreversibility of the refrigerant condenser could be reduced by decreasing the refrigerant pressure in the low-pressure leg to bring the condensing pressure closer to 20°C (but at the cost of additional condenser surface area). Most of the internal irreversibilities of the mechanical components are small relative to those of the heat transfer processes, as is usually the case. Note that the 100°C liquid water exhaust has very little useful work potential left. Also note that the helium heat exchanger is nicely balanced with a small ΔT , giving a low irreversibility. This is what the whole system should look like with good design.

ME 430/599C – Advanced Energy
Problem Set 3 – Assigned October 8, Due Friday, October 12, 4:30PM

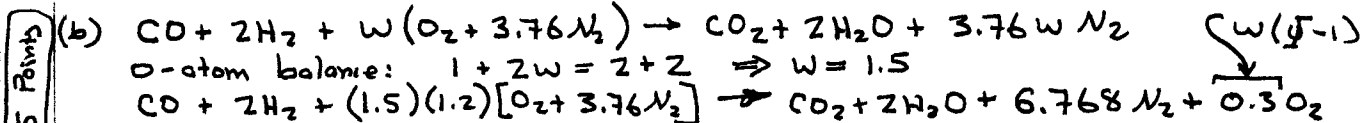
The following problems should be solved by hand, not using the equilibrium code.

1. Find the mole fraction (dry) for CO_2 and O_2 in the dried product gas of combustion fueled by the following:
 - (a) $\text{C}_8\text{H}_{18} + 20\%$ excess air
 - (b) $\text{CO} + 2\text{H}_2 + 20\%$ excess air (the represents a biomass gasification product)
2. During cold spells in the winter the very high natural gas demand for home heating in Seattle can stretch pipeline delivery capacity. Because of this, large users (such as the UW power plant), are supplied on an interruptible basis. In return for a lower gas rate, they agree to allow their supply to be shut off during these very high demand periods. Our power plant has large underground storage tanks of fuel oil (under the concrete parking lot on the south side of the complex) for use during these episodes. Assume the plant is burning fuel oil with the same composition as decane ($\text{C}_{10}\text{H}_{22}$), and that the mole fraction of O_2 in the exhaust is measured as 4.0% by a hot oxygen sensor (this would be wet basis as the sensor is hot enough to avoid condensation problems). Find the percent theoretical air.
3. 1 kg of C_2H_4 is burned with 30% excess air in a non-adiabatic flow combustor. The reactants are at 298 K and 1 atm. Enough heat is removed to cool the products to 800 K. Find the amount of heat removed (kJ)
4. C_2H_4 is burned with an unknown amount of air (reactants at 298 K and 1 atm.) in an adiabatic combustor. The product gases are found to be at 800 K. Find the percent excess air.



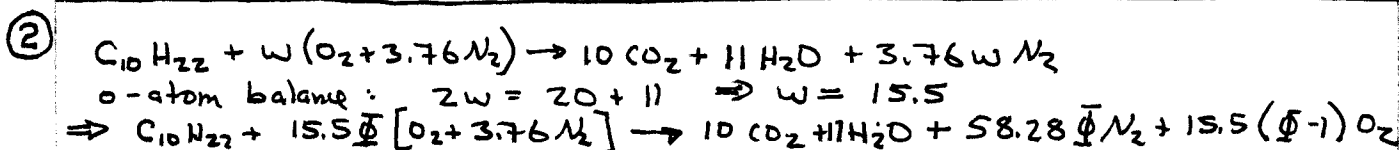
$$y_{CO_2} = \frac{n_{CO_2}}{\sum n_i - n_{H_2O}} = \frac{8}{8 + 56.4 + 2.5} \Rightarrow y_{CO_2} = 0.1196$$

$$y_{O_2} = \frac{n_{O_2}}{\sum n_i - n_{H_2O}} = \frac{2.5}{8 + 56.4 + 2.5} \Rightarrow y_{O_2} = 0.0374$$



$$y_{CO_2} = \frac{n_{CO_2}}{\sum n_i - n_{H_2O}} = \frac{1}{1 + 6.768 + 0.3} \Rightarrow y_{CO_2} = 0.1239$$

$$y_{O_2} = \frac{n_{O_2}}{\sum n_i - n_{H_2O}} = \frac{0.3}{1 + 6.768 + 0.3} \Rightarrow y_{O_2} = 0.0372$$



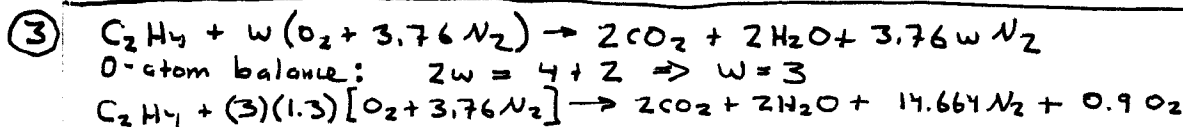
$$y_{O_2} = \frac{n_{O_2}}{\sum n_i} = \frac{15.5\phi - 15.5}{10 + 11 + 58.28\phi + 15.5\phi - 15.5} = \frac{15.5\phi - 15.5}{73.78\phi + 5.5}$$

$$73.78\phi y_{O_2} + 5.5y_{O_2} = 15.5\phi - 15.5$$

$$\phi [73.78y_{O_2} - 15.5] = -5.5y_{O_2} - 15.5$$

$$\Rightarrow \phi = \frac{-5.5y_{O_2} - 15.5}{73.78y_{O_2} - 15.5} = \frac{-(5.5)(0.04) - 15.5}{(73.78)(0.04) - 15.5} = \frac{1.2526}{1.2176}$$

$$\Rightarrow 125.26\% \text{ Theoretical Air}$$



$Q = H_P - H_R$

Species	$\frac{Kmoles}{Species}$	h_f°	$h - h_{298}$	$n_i [h_f^\circ + h - h_{298}]$	
C_2H_4	1	+52,280	0	+52,280	$H_R =$ +52,280
O_2	3.9	0	0	0	
N_2	14.664	0	0	0	
CO_2	2	-393,520	32,179 - 9364	-741,410	$H_P =$ -954,189
$H_2O(g)$	2	-241,820	23,896 - 9904	-447,656	
N_2	14.664	0	23,714 - 8669	+220,620	
O_2	0.9	0	24,523 - 8682	+14,257	

$$Q = H_P - H_R = -954,189 - 52,280 = -1,006,469.$$

-1,006,469 kJ	Kmole C_2H_4	1 kg C_2H_4	$\Rightarrow Q = -35,876 \text{ kJ}$
	28.054 kg C_2H_4		

④ From Problem 3: $C_2H_4 + 3\Phi [O_2 + 3.76 N_2] \rightarrow 2CO_2 + 2H_2O + 11.28\Phi N_2 + 3(\Phi - 1) O_2$

$H_R = H_P$

Species	Kmols	h_f°	$h - h_{298}$	$n_i (h_f^\circ + h - h_{298})$
C_2H_4	1	+52,280	0	+52,280.
O_2	3Φ	0	0	0
N_2	11.28Φ	0	0	0
CO_2	2	-393,520	32,179-9364	~~-714,410.~~ -741,410
H_2O	2	-241,820	27,896-9904	-447,656.
N_2	11.28Φ	0	23,714-8669	+169,708 Φ
O_2	$3\Phi - 3$	0	24,523-8682	+47,523 Φ - 47,523.

$H_R = +52,280.$

$$H_P = 217,231\Phi - 1,236,589.$$

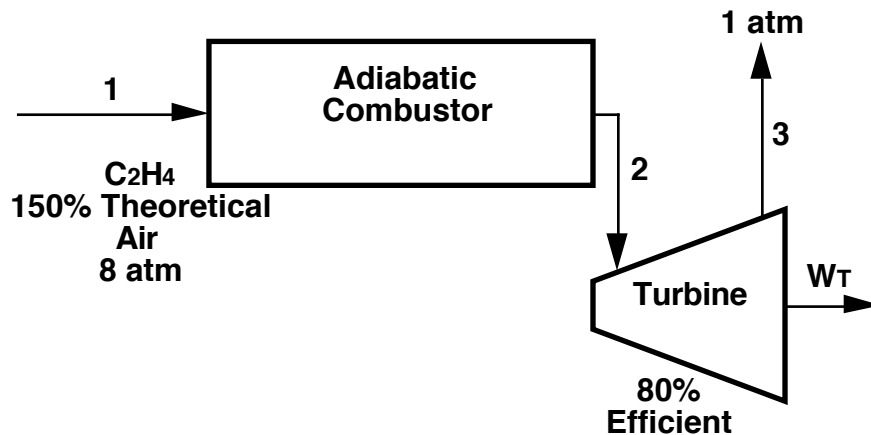
$$+52,280. = +217,231\Phi - 1,236,589.$$

$$\Rightarrow \Phi_{AF} = 5.9332 \Rightarrow \boxed{493.32\% \text{ Excess Air}}$$

5 Points

ME430/599C – Advanced Energy Systems
Problem Set 4: Assigned Oct. 9, Due Tuesday, Oct. 16, 4:30PM

1. Verify your answer to Problem 3 of Problem Set 3 using the equilibrium code. Specifically, use the code to find h for the products.
2. Verify your answer to Problem 4 of Problem Set 3 using the equilibrium code. Specifically, show that the stoichiometry calculated in Problem 4 yields 800 K as the product gas temperature when the code is run for an adiabatic problem.
3. Ethylene (C_2H_4) is burned with 150% theoretical air at 8 atm pressure (air and fuel arrive as a combined stream at 8 atm and 298 K). Find the adiabatic flame temperature using the equilibrium code. Also find the availability of the reactant stream and the irreversibility of the combustor (kJ/kmole ethylene). The dead state is 298 K, 1 atm.
4. The product gas from Problem 3 is expanded across an adiabatic turbine to 1 atm. The turbine efficiency is 80%. Making use of the equilibrium code, find:
 - (a) The outlet temperature (K) and enthalpy (kJ/kmole ethylene) if the turbine were behaving as isentropic.
 - (b) The actual outlet enthalpy (kJ/kmole ethylene) using the turbine efficiency equation.
 - (c) The actual outlet entropy (kJ/kmole ethylene) and temperature (K) using the code.
 - (d) The turbine irreversibility (kJ/kmole ethylene).
 - (e) The turbine work (kJ/kmole ethylene).
 - (f) The availability of the exhaust gas (kJ/kmole ethylene).
 - (g) Show that (d)+(e)+(f)+[combustor irreversibility] adds up to the availability from Problem 3. Note where the biggest losses of work potential occur. \



- ① Code was run as follows: $\left. \begin{array}{c} \text{C}_2\text{H}_4 \\ \text{air} \end{array} \right| \Phi_{FA} = 0.7692 \mid TP \mid \left. \begin{array}{c} T_f = 800 \text{ K} \\ P_f = 1 \text{ atm.} \end{array} \right\} h_f = -1692.833 \text{ KJ/kg}$
 $30\% \text{ EA} = 130\% \text{ TA} = \Phi_{AF} = 1.3$

5 Points

$$\text{C}_2\text{H}_4 + (3)(1.3)[\text{O}_2 + 3.76\text{N}_2] \rightarrow 28 \quad (3)(1.3)[32 + (3.76)(28)] = 563.39 \frac{\text{kg mix}}{\text{kmole C}_2\text{H}_4}$$

$$\Rightarrow h_f = \frac{-1692.833 \text{ KJ}}{\text{kg mix}} \mid \frac{563.39 \text{ kg mix}}{\text{kmole C}_2\text{H}_4} \Rightarrow h_f = -953,728 \frac{\text{KJ}}{\text{kmole C}_2\text{H}_4}$$

Compares to $\Rightarrow -954,189$
 Since rest of problem is the same, the answer is verified.

- ② This is an adiabatic problem where we vary Φ_{FA} until we hit a product T of 800K.

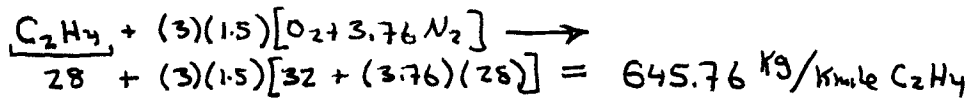
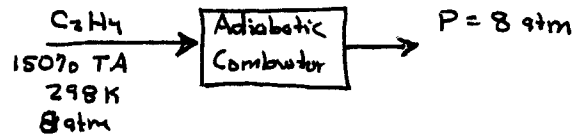
5 Pts

$$\left. \begin{array}{c} \text{C}_2\text{H}_4 \\ \text{air} \end{array} \right| \Phi_{FA} = \text{vary} \mid HP \mid \left. \begin{array}{c} T_i = 298 \text{ K} \\ P_i = 1 \text{ atm} \end{array} \right\} \left. \begin{array}{c} \Phi_{FA} \rightarrow T_p (\text{K}) \\ 0.5 \quad 800. \\ 0.25 \quad 1016. \\ 0.15 \quad 748. \\ 0.1694 \quad 802.34 \\ 0.1686 \quad 800.15 \leftarrow \text{OK} \end{array} \right\}$$

$$\Phi_{AF} = \frac{1}{0.1686} = 5.9312 \Rightarrow \boxed{493.12\% \text{ Theoretical Air}}$$

Matches 493.32% from Problem 4

- ③ First need h and s for reactants:



Species	Kmols	h_i°	$h - h_{298}$	S_i°	P_i	S_i
C ₂ H ₄	1	+52,280	0	219.83	0.3568	228.40
O ₂	4.5	0	0	205.04	1.6057	201.10
N ₂	16.92	0	0	191.61	6.0375	176.66
$n_T = 22.42$						

$S_i = \sum n_i S_i = 4122.43 \frac{\text{KJ}}{\text{kmole} \cdot \text{K}}$

$h_i = +52,280 \frac{\text{KJ}}{\text{kmole}}$

$P_i = \frac{n_i}{n_T} P = \frac{n_i}{22.42} (8 \text{ atm})$

$S_i = S_i^\circ - R \ln \frac{P_i}{P^\circ} = S_i^\circ - (8.314 \frac{\text{KJ}}{\text{kmole} \cdot \text{K}}) \ln \left(\frac{P_i}{1} \right)$

10 Points

Next run code: $\left. \begin{array}{c} \text{C}_2\text{H}_4 \\ \text{air} \end{array} \right| \Phi_{FA} = 0.667 \mid HP \mid \left. \begin{array}{c} T_i = 298 \text{ K} \\ P_i = 8 \text{ atm.} \end{array} \right\} \Rightarrow \boxed{T_p = 1939.69 \text{ K}}$

$h_p = 81.108 \frac{\text{KJ}}{\text{kg}}$
 $S_p = 8.6043 \frac{\text{KJ}}{\text{kg} \cdot \text{K}}$

$h_p = \frac{81.108 \text{ KJ}}{\text{kg}} \mid \frac{645.76 \text{ kg}}{\text{kmole C}_2\text{H}_4} = 52,376 \text{ KJ/kmole C}_2\text{H}_4 (= h_R)$

$$S_p = \frac{8.6043 \text{ KJ}}{\text{kg} \cdot \text{K}} \mid \frac{645.76 \text{ kg}}{\text{kmole C}_2\text{H}_4} = 5556.31 \text{ KJ/kmole} \cdot \text{K}$$

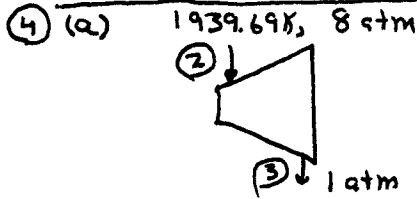
Next, run code for dead state $\left. \begin{array}{c} \text{C}_2\text{H}_4 \\ \text{air} \end{array} \right| \Phi_{FA} = 0.667 \mid TP \mid \left. \begin{array}{c} T_f = 298 \text{ K} \\ P_f = 1 \text{ atm} \end{array} \right\} = \left. \begin{array}{c} h_o = -1967.922 \text{ KJ/kg} \\ = -1,270,805 \text{ KJ/kmole} \\ S_o = 6.9748 \text{ KJ/kg} \cdot \text{K} \\ = 4504.05 \text{ KJ/kmole} \cdot \text{K} \end{array} \right\}$

$$W_{max} = h_1 - h_0 - T_0(S_1 - S_0) = 52,280 - [-1,270,805] \frac{\text{kJ}}{\text{kmole}} - (298\text{K}) [4122.43 - 4504.05 \frac{\text{kJ}}{\text{kmole-K}}]$$

$$\Rightarrow W_{max} = 1,436,808 \text{ kJ/kmole } C_2H_4$$

$$i_{comb} = T_0(S_P - S_R) = (298\text{K}) [5556.31 - 4122.43 \frac{\text{kJ}}{\text{kmole-K}}]$$

$$\Rightarrow i_{comb} = 427,296 \text{ kJ/kmole } C_2H_4$$



Code: $\frac{C_2H_4}{air} \bigg| \Phi_{FA} = 0.667 \bigg| TP \bigg| P = 1 \text{ atm}$
 $T = \text{Guess until } S = 8.6043 \text{ kJ/kg-K}$

$T_P (\text{K})$	$S_P (\text{kJ/kg-K})$
1200	8.5587
1300	8.6616
1244	8.6048

$\Rightarrow T_{3,S} = 1244 \text{ K} \Rightarrow h_{3,S} = -861.565 \frac{\text{kJ}}{\text{kg}}$

(b) $\eta_T = \frac{W_T}{W_S} = \frac{h_2 - h_3}{h_2 - h_{3,S}} \Rightarrow 0.8 = \frac{81.108 - h_3}{81.108 - (-861.565)}$

$$\Rightarrow h_3 = -673.10 \frac{\text{kJ}}{\text{kg}} \Rightarrow h_3 = -434,663 \frac{\text{kJ}}{\text{kmole } C_2H_4}$$

(c) Run code: $\frac{C_2H_4}{air} \bigg| \Phi_{FA} = 0.667 \bigg| TP \bigg| P = 1 \text{ atm}$
 $T = \text{guess}$ } iterate until $h_P = h_3$ above

$T (\text{K})$	$h (\text{kJ/kg})$
1300	-789.263
1400	-658.596
1388.9	-673.202 ← OK

$T_3 = 1388.9 \text{ K}$

$\Rightarrow S_3 = 8.7480 \text{ kJ/kg-K} \Rightarrow S_3 = 5649.11 \text{ kJ/kmole } C_2H_4$

(d) $i_T = T_0(S_3 - S_2) = (298\text{K}) [5649.11 - 5556.31 \frac{\text{kJ}}{\text{kmole-K}}]$

$i_T = 27,654 \text{ kJ/kmole } C_2H_4$

(e) $W_T = h_2 - h_3 = 52,376 - (-434,663) \frac{\text{kJ}}{\text{kmole}}$
 $\Rightarrow W_T = 487,039 \frac{\text{kJ}}{\text{kmole } C_2H_4}$

(f) $W_{lost} = h_3 - h_0 - T_0(S_3 - S_0) = -434,663 - (-1,270,805) \frac{\text{kJ}}{\text{kmole}} - (298\text{K}) [5649.11 - 4504.05 \frac{\text{kJ}}{\text{kmole-K}}]$
 $\Rightarrow W_{lost} = 494,914 \text{ kJ/kmole } C_2H_4$

(g)

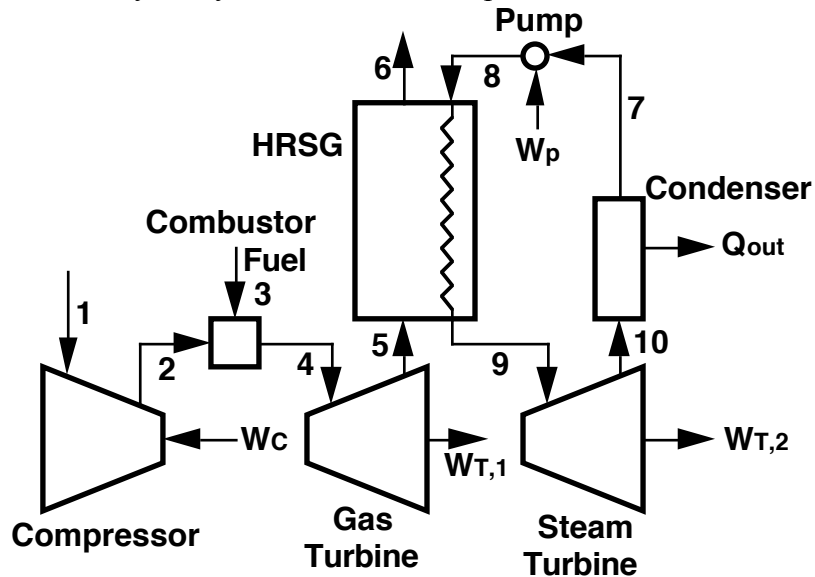
Item	$\frac{\text{kJ}}{\text{kmole } C_2H_4}$	T_0
Availability	1,436,808	100.0
$W_{lost} @ \text{exhaust}$	494,914	34.4
W_T	487,039	33.9
i_{comb}	427,296	29.7
i_T	27,654	1.9
Σ	1,436,903	Closes to 0.00770 %

The big losses

Address the lost work at exhaust via bottoming cycle. Address combustor irreversibility via fuel cell.

ME430/599C – Advanced Energy Systems
Problem Set 5: Assigned Oct. 15, Due Friday, Oct. 19, 4:30PM

This problem set relates to the gas turbine part of a combined cycle system. Consider the system shown below. The air enters the system at 1 atm pressure and 298 K. The compressor has an adiabatic efficiency of 85%. The combustor is adiabatic, and the fuel (methane) arrives at 298 K and the compressor outlet pressure. Enough fuel is added to take the combustor outlet temperature to 1600 K. The turbine has an adiabatic efficiency of 85% and discharges at 1 atm. As discussed in class, the only really free variable is the pressure ratio.



1. Assume the pressure ratio is 28. Find T_5 (I got 864 K). Note that this requires you to find the combustor stoichiometry. Use the equilibrium code and variable specific heat treatment on the compressor air.
2. Find the availability of the inlet streams on a /kg air basis. Then find the net work, the irreversibilities in the compressor, combustor, and gas turbine, and the lost work at 5 (all /kg air). These should sum to the availability.

Note that close attention to units is critical to developing a consistent analysis. You have three flows in this system: air flow, fuel flow, and product gas flow. Also, anything that you calculate on a basis of /kmole CH_4 needs to be converted to the correct basis.

① Air compressor: $T_1 = 298 \text{ K} \Rightarrow h_1 = 298.18 \text{ kJ/kg}$, $P_{r,1} = 1.3543$, $S_1^\circ = 1.69528 \text{ kJ/kg-K}$

$$P_{r,2} = P_{r,1} \left[\frac{P_2}{P_1} \right] = (1.3543)(28) = 37.9204 \Rightarrow h_{2,s} = 770.53 \text{ kJ/kg}$$

$$\eta_c = \frac{w_s}{w_a} = \frac{h_{2,s} - h_1}{h_2 - h_1} \Rightarrow 0.85 = \frac{770.53 - 298.18}{h_2 - 298.18} \Rightarrow 853.88 \text{ kJ/kg}$$

$$\Rightarrow T_2 = 828.96 \text{ K}, S_2^\circ = 2.7570 \text{ kJ/kg-K}$$

Combustor: $\left. \begin{array}{l} \frac{\text{CH}_4}{\text{air}} \mid \Phi_{FA} = \text{vary} \mid \text{HP} \mid \begin{array}{l} T_{\text{fuel}} = 298 \text{ K} \\ T_{\text{air}} = 828.96 \text{ K} \end{array} \right\} \text{ Vary } \Phi \text{ until } T_4 = 1600 \text{ K}$

Φ_{FA}	$T(\text{K})$
0.5	1874.14
0.33	1501.44
0.3529	1605.13
0.3503	1600.12

$$\Rightarrow \Phi_{AF} = 1/\Phi_{FA} = 1/0.3503 = 2.855$$

$$\Rightarrow h_4 = 454.499 \text{ kJ/kg mix}, S_4 = 8.0140 \text{ kJ/kg mix-K}$$

Now do stoichiometry to get correct mass basis: $\text{CH}_4 + [2][2.855][\text{O}_2 + 3.76 \text{ N}_2]$
 mass: 16 (2)(2.855)[32 + (3.76)(28)]

$$m_f = 16 \text{ mox} = 783.87$$

$$\Rightarrow m_p = 799.87 \text{ kg}$$

Using a basis of 1 kg air $\Rightarrow m_f = 0.0204 \text{ kg fuel/kg air}$
 $m_p = 1.0204 \text{ kg product/kg air}$

Next assume turbine is isentropic:

$\left. \begin{array}{l} \frac{\text{CH}_4}{\text{air}} \mid \Phi_{FA} = 0.3503 \mid \text{TP} \mid \begin{array}{l} P_t = 1 \text{ atm} \\ T_t = \text{guess} \end{array} \right\} \text{ Vary } T_t \text{ until } S_5 = S_4$

$T(\text{K})$	S
742.	8.0429
700.	7.9765
723.7	8.0143

$$\Rightarrow h_{5,s} = -633.565 \text{ kJ/kg}$$

Apply turbine efficiency calc: $\eta_T = \frac{w_t}{w_s} = \frac{h_4 - h_5}{h_4 - h_{5,s}} \Rightarrow 0.85 = \frac{454.499 - h_5}{454.499 - (-633.565)}$

$$\Rightarrow h_5 = -470.355 \text{ kJ/kg}$$

Now use code in TP mode to find turbine outlet condition that corresponds to h_5 .

$\left. \begin{array}{l} \frac{\text{CH}_4}{\text{air}} \mid \Phi_{FA} = 0.3503 \mid \text{TP} \mid \begin{array}{l} P_t = 1 \text{ atm} \\ T_t = \text{guess} \end{array} \right\} \text{ Vary } T_t \text{ until you get } h_5$

$T(\text{K})$	h
850.	-487.394
875.	-457.959
864.5	-470.345

$$\Rightarrow T_5 = 864.5 \text{ K}, S_5 = 8.2203 \text{ kJ/kg mix-K}$$

② Inlet streams:

Species	Kmoles	h_f°	$h - h_{298}$	S_i°	$P_i (\text{atm})$	S_i
CH ₄	1	-74,850	0	186.16	28	158.47
O ₂	5.71	0	0	205.04	0.21	218.12
N ₂	21.47	0	0	191.61	0.79	193.57

$h = -74,850 \text{ kJ/kmole CH}_4$

$\left. \begin{array}{l} \sum n_i S_i = S = 5559.88 \frac{\text{kJ}}{\text{kmole-K CH}_4} \end{array} \right\}$

$$\text{Converting: } h = \frac{-74,850 \text{ kJ}}{\text{kmole CH}_4} \mid \frac{7 \text{ kmole CH}_4}{783.87 \text{ kg air}} = -95.49 \text{ kJ/kg air}$$

(2)

$$S = \frac{5559.88 \text{ kJ}}{\text{kmole CH}_4 \cdot \text{K}} \left| \frac{1 \text{ kmole CH}_4}{783.87 \text{ kg air}} \right| = 7.0929 \text{ kJ/kg air} \cdot \text{K}$$

Dead state from code:

$$\left. \begin{array}{l} \text{CH}_4 \\ \text{air} \end{array} \right| \Phi_{FA} = 0.3503 \left| \text{TP} \right| \left. \begin{array}{l} P = 1 \text{ atm} \\ T = 298 \text{ K} \end{array} \right\} \Rightarrow \begin{array}{l} h_0 = -1096.438 \text{ kJ/kg mix} \\ S_0 = 7.0555 \text{ kJ/g} \cdot \text{K} \end{array}$$

Converting:

$$h_0 = \frac{-1096.438 \text{ kJ}}{\text{kg mix}} \left| \frac{1.0204 \text{ kg mix}}{\text{kg air}} \right| = -1118.80 \text{ kJ/kg air}$$

$$S_0 = \frac{7.0555 \text{ kJ}}{\text{kg mix} \cdot \text{K}} \left| \frac{1.0204 \text{ kg mix}}{\text{kg air}} \right| = 7.1994 \text{ kJ/kg air} \cdot \text{K}$$

$$W_{\max} = h - h_0 - T_0 (S - S_0) = -95.49 - (-1118.80) - (298 \text{ K})(7.0929 - 7.1994) \\ \Rightarrow W_{\max} = 1055.06 \text{ kJ/kg air}$$

$$W_{\text{net}} = m_p (h_4 - h_5) - m_a (h_2 - h_1) = (1.0204) \left(\frac{\text{kg mix}}{\text{kg air}} \right) (454.499 - (-470.355 \frac{\text{kJ}}{\text{kg mix}})) \\ - (1 \text{ kg air}) \left[853.88 - 298.18 \frac{\text{kJ}}{\text{kg air}} \right] \\ \Rightarrow W_{\text{net}} = 388.02 \text{ kJ/kg air}$$

$$i_{\text{comp}} = T_0 (S_2 - S_1) = T_0 (S_2^0 - S_1^0 - R \ln \frac{P_2}{P_1}) \\ = (298 \text{ K}) \left[2.7570 - 1.69528 \frac{\text{kJ}}{\text{kg air} \cdot \text{K}} - (0.287 \frac{\text{kJ}}{\text{kg air} \cdot \text{K}}) \ln(28) \right] \\ \Rightarrow i_{\text{comp}} = 31.40 \text{ kJ/kg air}$$

Need S_{in} for combustor:

Species	Kmole	S_i^0	P_i	S_i
CH ₄	1	186.16	28.	158.46
O ₂	5.71	237.01	5.88	222.28
N ₂	21.47	222.03	22.12	196.28

$$S = \sum n_i S_i = 5641.94 \frac{\text{kJ}}{\text{kmole CH}_4 \cdot \text{K}}$$

$$\text{Converting: } S_R = \frac{5641.94 \text{ kJ}}{\text{kmole CH}_4 \cdot \text{K}} \left| \frac{1 \text{ kmole CH}_4}{783.87 \text{ kg air}} \right| = 7.1975 \frac{\text{kJ}}{\text{kg air} \cdot \text{K}}$$

$$S_4 = \frac{8.0140 \text{ kJ}}{\text{kg mix} \cdot \text{K}} \left| \frac{1.0204 \text{ kg mix}}{\text{kg air}} \right| = 8.1775 \frac{\text{kJ}}{\text{kg air} \cdot \text{K}}$$

$$i_{\text{comb}} = T_0 (S_4 - S_R) = (298 \text{ K})(8.1775 - 7.1975 \frac{\text{kJ}}{\text{kg air} \cdot \text{K}})$$

$$i_{\text{comb}} = 292.04 \text{ kJ/kg air}$$

$$\text{Turbine: } i_T = T_0 (S_5 - S_4) = \frac{298 \text{ K} \left[8.2203 - 8.0140 \frac{\text{kJ}}{\text{kg mix} \cdot \text{K}} \right] \left| \frac{1.0204 \text{ kg mix}}{\text{kg air}} \right|}{\text{kg air}}$$

$$i_T = 62.73 \text{ kJ/kg air}$$

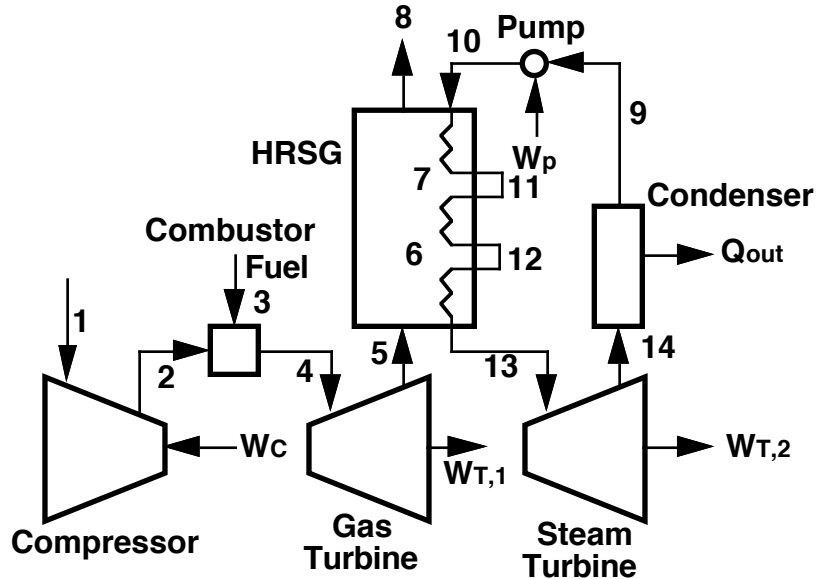
$$\text{Lost work @ } S: h_5 = \frac{-470.355 \text{ kJ}}{\text{kg mix}} \left| \frac{1.0204 \text{ kg mix}}{\text{kg air}} \right| = -479.95 \text{ kJ/kg air}$$

$$W_{\max} = h_5 - h_0 - T_0 (S_5 - S_0) = -479.95 - (-1118.80) - (298 \text{ K}) \left[\frac{8.2203 \text{ kJ}}{\text{kg mix} \cdot \text{K}} \left| \frac{1.0204 \text{ kg mix}}{\text{kg air}} \right| - 7.1994 \frac{\text{kJ}}{\text{kg air} \cdot \text{K}} \right] \\ \Rightarrow W_{\text{lost}, S} = 284.65 \text{ kJ/kg air}$$

$$\text{Check: } W_{\text{net}} + i_{\text{comp}} + i_{\text{comb}} + i_{\text{Turb}} + W_{\text{lost}, S} = 388.02 + 31.40 + 292.04 + 62.73 + 284.65 \\ = 1058.84 \text{ kJ/kg air (within 0.36\%)}$$

ME430/599C – Advanced Energy Systems
Problem Set 6: Assigned Oct. 15, Due Monday, Oct. 22, 4:30PM

We continue with our analysis of a basic combined cycle system. The properties of the gas turbine cycle are the same as given in Problem Set 5, and values from that solution set can be used directly here.. We will continue to use the per kg air basis. The properties of the steam cycle are as follows: condenser pressure: 5 kPa, condenser outlet: saturated liquid, boiler pressure: 10 MPa, pump is isentropic, turbine efficiency: 80%, steam superheat temperature is 50 K below T_5 . Assume the minimum ΔT for heat transfer in the HRSG (the limiting condition point) is 10 K. The environment is at 298 K and 1 atm.



1. Find the steam flow (kg steam/kg air)
2. Complete the thermodynamic analysis of the cycle and present your results in a table. This should include the total net work (sum of steam and gas turbine cycles, each irreversibility, and any lost work associated with exit flows. It should cover the entire combined cycle, but again you do not need to rework the gas turbine part. The table should show kJ/kg air and percentage of total original availability and should be ordered from highest to lowest value. Again, the basis is 1 kg air into the gas turbine compressor. You will need to use the code to get correct properties for the needed combustion gas points in the HRSG.

① First get the steam cycle properties:

$$\textcircled{9} \text{ Sat. Liq. } 5 \text{ kPa} \Rightarrow h_9 = 137.75 \text{ kJ/kg}, S_9 = 0.4762 \text{ kJ/kg-K}$$

$$v_9 = 1.005 \text{ E-3 m}^3/\text{kg}, T_9 = 32.87^\circ\text{C}$$

$$\textcircled{10} W_p = v_9 (P_0 - P_9) = \frac{1.005 \text{ E-3 m}^3}{\text{kg}} | 10,000 - 5 \text{ kPa} = 10.04 \text{ kJ/kg St.}$$

$$h_{10} = h_9 + W_p = 137.75 + 10.04 \text{ kJ/kg St} = 147.79 \text{ kJ/kg St}$$

$$T_{10} = T_9, S_{10} = S_9$$

$$\textcircled{13} T_5 = 864 \text{ K} \Rightarrow T_{13} = T_5 - 50 \text{ K} = 864 \text{ K} - 50 \text{ K} = 814 \text{ K} = 541^\circ\text{C}$$

$$P_{13} = 10 \text{ MPa} \Rightarrow h_{13} = 3479.2 \text{ kJ/kg St}, S_{13} = 6.7299 \text{ kJ/kg St-K}$$

$$\textcircled{14} P_{14} = 5 \text{ kPa}, S_{14} = S_{13} \Rightarrow \text{Sat mix}$$

$$X_{14,5} = \frac{6.7299 - 0.4762}{7.9176} = 0.7898$$

$$h_{14,5} = h_f + X_{14,5} h_{fg} = 137.75 + [0.7898][2423.0] = 2051.5 \text{ kJ/kg St}$$

$$\eta_T = \frac{W_a}{W_s} = \frac{h_{13} - h_{14}}{h_{13} - h_{14,5}} \Rightarrow 0.8 = \frac{3479.2 - h_{14}}{3479.2 - 2051.5} \Rightarrow h_{14} = 2337.1 \text{ kJ/kg St}$$

Now actual quality and S_{14} : $X_{14} = \frac{h_{14} - h_f}{h_{fg}} = \frac{2337.1 - 137.75}{2423} = 0.9077$

$$S_{14} = S_f + X_{14} S_{fg} = 0.4762 + [0.9077][7.9176] = 7.6630 \text{ kJ/kg St-K}$$

$$\textcircled{11} \text{ Sat Liq. } 10 \text{ MPa} \Rightarrow h_{11} = 1407.8 \text{ kJ/kg St}, S_{11} = 3.3603 \text{ kJ/kg St-K}$$

$$T_{11} = 311.0^\circ\text{C} = 584 \text{ K}$$

Because of low T_5 , assume PP is controlling, 1st Law on SH + Boiler.

$$\text{Assume } T_7 = T_{11} + 10 = 584 \text{ K} + 10 \text{ K} = 594 \text{ K}$$

Now get h_7 from code.

$$\left. \begin{array}{l} \text{CH}_4 \\ \text{air} \end{array} \right| \Phi_{FA} = 0.3503 \left| \begin{array}{l} TP \\ T = 594 \text{ K} \end{array} \right| P = 1 \text{ atm} \left\} h_7 = -779.057 \text{ kJ/kg mix}$$

$$\text{Converting: } \frac{-779.057 \text{ kJ}}{\text{kg mix}} \left| \frac{1.0204 \text{ kg mix}}{\text{kg air}} \right. \Rightarrow h_7 = -794.95 \text{ kJ/kg air}$$

$$\Rightarrow m_a (h_5 - h_7) = m_{st} (h_{13} - h_{11})$$

$$(1) \frac{(-779.057 - (-794.95))}{\text{kJ/kg air}} = m_{st} (3479.2 - 1407.8 \text{ kJ/kg St})$$

$$\Rightarrow m_{st} = 0.1521 \frac{\text{kg St}}{\text{kg air}}$$

② Now check exit condition: 1st Law on FWH

$$m_a (h_7 - h_8) = m_{st} (h_{11} - h_{10})$$

$$(1 \text{ kg air}) (-794.95 - h_8 \text{ kJ/kg air}) = (0.1521 \text{ kg St}) (1407.8 - 147.79 \text{ kJ/kg St})$$

$$\Rightarrow h_8 = -986.60 \text{ kJ/kg air}$$

$$\text{Converting: } \frac{-986.60 \text{ kJ}}{\text{kg air}} \left| \frac{1.0204 \text{ kg mix}}{\text{kg air}} \right. \Rightarrow h_8 = -966.87 \frac{\text{kJ}}{\text{kg mix}}$$

Now run code to find T_8, S_8

$$\left. \begin{array}{l} \text{CH}_4 \\ \text{air} \end{array} \right| \Phi_{FA} = 0.3503 \left| \begin{array}{l} TP \\ T = \text{guess} \end{array} \right| P = 1 \text{ atm}$$

Guess T until h_8 matches.

T (K)	h
425	-962.323
420	-967.633

$$T_8 = 420.72 \quad \frac{-966.88}{\text{OK}} \Rightarrow S_8 = 7.4194 \text{ kJ/kg mix-K}$$

10 Points

15 Points

Checking $T_8 - T_{10} = 420.72 - (32.87 + 273K) = 115K$ so we are OK.

Converting: $S_8 = \frac{7.4194 \text{ KJ}}{\text{kg mix} \cdot K} \bigg| \frac{1.0204 \text{ kg mix}}{1.0204 \text{ kg air}} = 7.5708 \text{ KJ/kg air} \cdot K$

Now pull it together:

$$W_{\text{net, Rankine}} = m_{st} [h_{13} - h_{14} - W_P] = (0.1521 \frac{\text{kg st}}{\text{kg air}}) [3479.2 - 2337.1 - 10.04 \frac{\text{KJ}}{\text{kg st}}]$$

$$W_{\text{Rank}} = 172.19 \text{ KJ/kg air}$$

$$i_{\text{HXSG}} = T_0 [m_a (S_8 - S_5) + m_{st} (S_{13} - S_{10})]$$

$$= (298K) \left[(1 \frac{\text{kg}}{\text{kg}}) (7.5708 - 8.3880 \frac{\text{KJ}}{\text{kg air} \cdot K}) + (0.1521 \frac{\text{kg st}}{\text{kg air}}) (6.7279 - 0.4762 \frac{\text{KJ}}{\text{kg st} \cdot K}) \right]$$

$$\frac{8.2203 \text{ KJ}}{\text{kg mix} \cdot K} \bigg| \frac{1.0203 \text{ kg mix}}{\text{kg air}} \Rightarrow i_{\text{HXSG}} = 39.93 \text{ KJ/kg air}$$

$$i_T = T_0 m_{st} (S_{14} - S_{13}) = (298K) (0.1521 \frac{\text{kg st}}{\text{kg air}}) (7.6630 - 6.7279 \frac{\text{KJ}}{\text{kg st} \cdot K})$$

$$i_T = 42.29 \text{ KJ/kg air}$$

Condenser: $q_{\text{out}} = h_{14} - h_9 = 2337.1 - 137.75 \text{ KJ/kg st} = 2199.35 \frac{\text{KJ}}{\text{kg st}}$

$$i_{\text{cond}} = T_0 m_{st} \left[S_9 - S_{14} + \frac{q_R}{T_R} \right] = (298K) (0.1521 \frac{\text{kg st}}{\text{kg air}}) \left[0.4762 - 7.6630 \frac{\text{KJ}}{\text{kg st} \cdot K} + \frac{2199.35 \text{ KJ/kg st}}{298K} \right]$$

$$i_{\text{cond}} = 8.77 \text{ KJ/kg air}$$

Lost work at (8): $W_{\text{lost}} = h_8 - h_0 - T_0 (S_8 - S_0)$

$$W_{\text{lost}} = -986.60 - (-1118.8) \frac{\text{KJ}}{\text{kg air}} - (298K) [7.5708 - 7.1994 \frac{\text{KJ}}{\text{kg air} \cdot K}]$$

$$W_{\text{lost}} = 21.52 \text{ KJ/kg air}$$

Finally $W_{\text{net}} = W_B + W_R = 388.02 + 172.19 \frac{\text{KJ}}{\text{kg air}} = 560.21 \text{ KJ/kg air}$

Just for interest, let's get the standard efficiency based on CH₄ LHV

560.21 KJ	783.87 kg air	Kmole CH ₄	kg CH ₄	100%
kg air	Kmole CH ₄	16 kg CH ₄	LHV = 50,050 KJ	= 54.8%

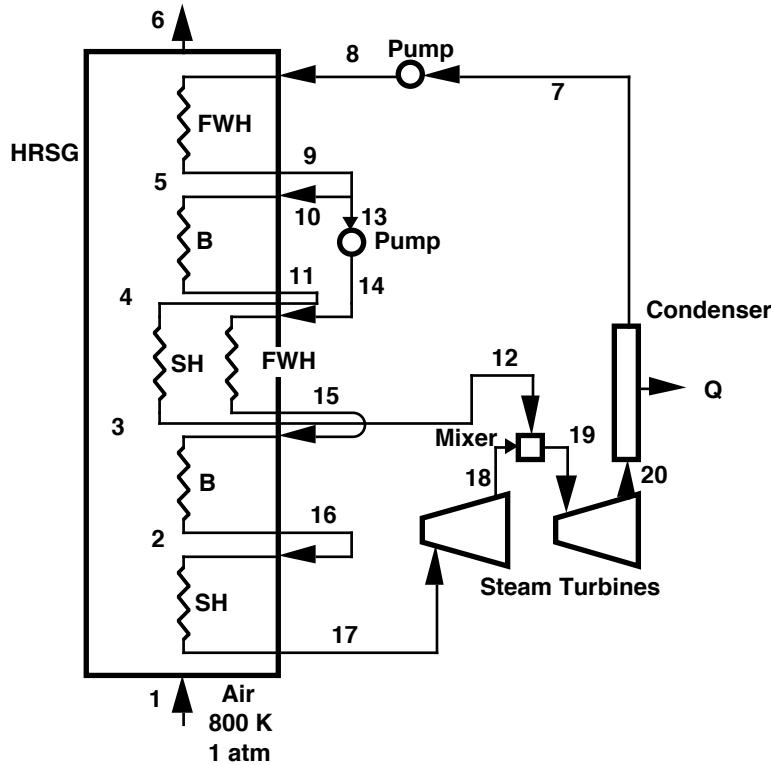
Item	kJ/kg air	Percent
Availability	1055.06	100.00
Net Work	560.21	52.91
I,comb	292.04	27.58
I,gas turbine	62.73	5.92
I,steam turbine	42.29	3.99
I,HRSG	39.93	3.77
I,comp	31.4	2.97
W,lost at 8	21.52	2.03
I,cond	8.77	0.83
Sum =	1058.89	
Closure, Percent	0.36	

The results show a 53% recovery of our availability. To squeeze any more out would require improving component efficiency (compressors and turbines) and working to reduce HRSG irreversibility by moving to a multi-pressure system. The very low condenser pressure has almost eliminated its irreversibility. Obviously, the combustor is the remaining bad player here. We can reduce its i a little by increasing our turbine inlet temperature closer to 1700 K. To reach 60% efficiency requires that we move about 75 kJ/kg air into the net work term from the various losses.

ME 430 – Advanced Energy

Problem Set 7: Assigned October 23, Due Wednesday, October 31, 4:30pm

- The following diagram shows a two-pressure steam cycle in a combined cycle system. This differs from that presented in class in that we superheat the low-pressure leg here.



To simplify the calculation, we will assume that the gas entering the HRSG from the gas turbine cycle (*i.e.*, Point 1) can be treated as air (800 K, 1 atm.). Furthermore, we will treat the air as a constant specific heat fluid throughout the calculation with $C_p = 1.0 \text{ kJ/kg-K}$ (*i.e.*, $h_1 - h_2 = C_p(T_1 - T_2)$); note that you have no reason to use the air tables in this problem). The air flow is 1 kg/s.

The steam cycle properties are as follows. The outlet of the condenser is a saturated liquid at 5 kPa. The first pump is isentropic, with an outlet pressure of 500 kPa. The flow at Point 9 splits, with one portion (Point 10) being reintroduced to be boiled, superheated to 300°C, and sent to the mixer. The remainder (Point 13) is isentropically pumped to 15 MPa, heated to saturation, boiled, and superheated to 450°C (Point 17). Both steam turbines can be assumed isentropic to simplify the calculations, and the mixer is adiabatic.

This system has two pinch points, at Points 3 and 5. We want to design the system such that the ΔT at both these points is 10 K.

- Find the steam flow through the high-pressure leg of the system (Points 15-17). *Hint:* What specific 1st law helps you here?
- Find the steam flow through the low-pressure leg (Points 10-12). *Hint:* Another specific 1st law balance gets you exactly what you need! Note that between Points 3 and 4 both the high

pressure and low pressure legs are extracting heat in parallel. This will not create a problem for you if you can write appropriate valid 1st laws.

(c) Find h_{18} , h_{19} , h_{20} .

(d) Find the turbine work (I got 171.02 kW).

2. Compare the wholesale costs of generating electricity between a coal-fired Rankine cycle and a natural gas fired combined cycle (¢/kW-hr).

Rankine cycle: 600 MW_e, 37% efficiency, capital cost \$1300/kW_e, coal cost 1.5 \$/10⁶ Btu, 75% capacity factor.

Combined cycle: 400 MW_e, 60% efficiency, capital cost \$550/kW_e, gas cost 8 \$/10⁶ Btu, 90% capacity factor.

For both cycles, assume 30 year life and 5% interest. Note that we have not included operating costs associated with pollutant abatement for the coal plant, but we have included these capital costs in the \$1300/kW_e figure.

3. Obtain the Ultimate analysis for Centralia coal. Go to:

<http://energy.er.usgs.gov/coalqual.htm>

Set the report to be generated to "Proximate & Ultimate analysis", the state to "Washington" and the field to "Centralia". Then hit "Submit" *under step 1*. *Note:* The Ultimate analysis has two changes from the format presented in class: (1) the H and O numbers presented in the Ultimate analysis include the H and the O from the moisture, and (2) the basis for the Ultimate analysis is the raw coal, not the DAF. The heat of combustion is the Higher Heating Value (HHV).

The power plant itself is briefly described under:

<http://www.power-technology.com/projects/centralia/>

Note that the complex consists of two coal-fired Rankine units (670 MW_e each) and a more recently added combined cycle unit (248 MW_e).

Assume the Rankine plants operate at 20% excess air, the inlet flows are all at 298 K and 1 atm., and that the stack gas exits at 450 K. Find the heat given up by the combustion of 100 kg of raw coal. Note that $h - h_{298}$ for SO₂ can be approximated by $C_{p,SO_2}(T-298)$ where $C_{p,SO_2}=42.6$ kJ/kmole-K. The h_f° for SO₂ is -296,840 kJ/kmole. You will need to make use of the "Getting Enthalpy of Formation..." handout to do this calculation.

① Steam properties:

$$\textcircled{7} \text{ Sat. Liq. - 5 kPa} \Rightarrow h_f = 137.75 \text{ kJ/kg}, v_f = 1.005 \text{ E-3 m}^3/\text{kg}$$

$$\textcircled{8} w_p = v_f (P_8 - P_7) = \frac{1.005 \text{ E-3 m}^3}{\text{kg}} | 500 - 5 \text{ kPa} = 0.50 \text{ kJ/kg st.}$$

$$h_8 = h_f + w_p = 137.75 + 0.50 \text{ kJ/kg st} = 138.25 \text{ kJ/kg st.}$$

$$\textcircled{9} \text{ Sat. Liq. - 500 kPa} \Rightarrow h_9 = 640.09 \text{ kJ/kg st}, v_9 = 1.093 \text{ E-3 m}^3/\text{kg st}$$

⑩ Same as ⑨

$$T_9 = 151.83^\circ\text{C} = 425 \text{ K}$$

$$\textcircled{11} \text{ Sat. Vapor @ 500 kPa} \Rightarrow h_{11} = 2748.1 \text{ kJ/kg st}$$

$$\textcircled{12} 500 \text{ kPa}, 300^\circ\text{C} \Rightarrow h_{12} = 3064.6 \text{ kJ/kg st}$$

⑬ Same as ⑨

$$\textcircled{14} w_p = v_9 (P_{14} - P_9) = \frac{1.093 \text{ E-3 m}^3}{\text{kg}} | 15,000 - 500 \text{ kPa} = 15.85 \text{ kJ/kg st.}$$

$$h_{14} = h_{12} + w_p = 640.09 + 15.85 = 655.94 \text{ kJ/kg st}$$

$$\textcircled{15} \text{ Sat. Liq. - 15,000 kPa}$$

$$\Rightarrow h_{15} = 1610.3 \text{ kJ/kg st}, T_{15} = 342.16^\circ\text{C} = 615 \text{ K.}$$

$$\textcircled{16} \text{ Sat. Vapor - 15 MPa} \Rightarrow h_{16} = 2610.8 \text{ kJ/kg st}$$

$$\textcircled{17} 15 \text{ MPa}, 450^\circ\text{C} \Rightarrow h_{17} = 3157.9 \text{ kJ/kg st}, s_{17} = 6.1434 \text{ kJ/kg st-K.}$$

$$\textcircled{18} 500 \text{ kPa}, s_{18} = s_{17} \Rightarrow \text{Sat. mix.}$$

$$x_{18} = \frac{s_{18} - s_f}{s_{fg}} = \frac{6.1434 - 1.8604}{4.9603} = 0.8635$$

$$\Rightarrow h_{18} = h_f + x_{18} h_{fg} = 640.09 + [0.8635] [2108.0] \text{ kJ/kg st} =$$

$$\Rightarrow h_{18} = 2460.25 \text{ kJ/kg st}$$

This is as far as we can go without having steam flows.

(a) First law on segment ①-③

$$\dot{m}_a C_{p,a} (T_1 - T_3) = \dot{m}_{st,HP} (h_{17} - h_{15})$$

$$\text{Select } T_3 \text{ to get a } \Delta T = 10 \text{ K @ } \textcircled{3} \Rightarrow T_3 = T_{15} + 10 \text{ K} = 615 + 10 \text{ K} = 625 \text{ K}$$

Note that since $T_{12} = 300^\circ\text{C}$, this is colder than T_{15} and does not impact minimum pp ΔT of 10 K.

$$(1 \text{ kg/s})(1.0 \frac{\text{kJ}}{\text{kg-K}})(800 - 625 \text{ K}) = \dot{m}_{st,HP} (3157.9 - 1610.3 \text{ kJ/kg st})$$

$$\Rightarrow \dot{m}_{st,HP} = 0.1131 \text{ kg st/s}$$

(b) First law on segment ③-⑤

$$\dot{m}_a C_{p,a} (T_3 - T_5) = \dot{m}_{st,HP} (h_{15} - h_{14}) + \dot{m}_{st,LP} (h_{12} - h_{10})$$

$$\text{To meet the second pp limit, let } T_5 = T_9 + 10 \text{ K} = 425 + 10 = 435 \text{ K}$$

$$(1 \text{ kg/s})(1.0 \text{ kJ/kg-K})(625 - 435 \text{ K}) = (0.1131 \frac{\text{kg st}}{\text{s}})(1610.3 - 655.94 \frac{\text{kJ}}{\text{kg st}}) + \dot{m}_{st,LP} (3064.6 - 640.09 \frac{\text{kJ}}{\text{kg st}})$$

$$\Rightarrow \dot{m}_{st,LP} = 0.0338 \text{ kg st/s}$$

$$\dot{m}_{st} = \dot{m}_{st,HP} + \dot{m}_{st,LP} = 0.1131 + 0.0338 = 0.1469 \text{ kg st/s}$$

(c) First law on mixer:

$$\dot{m}_{st,HP} h_{18} + \dot{m}_{st,LP} h_{12} = \dot{m}_{st} h_{19}$$

$$(0.1131)(2460.25) + (0.0338)(3064.3) = (0.1469) h_{19} \Rightarrow h_{19} = 2599.2 \text{ kJ/kg st}$$

$$\Rightarrow \text{Sat mix} \Rightarrow x_{19} = \frac{h_{19} - h_f}{h_{fg}} = \frac{2599.2 - 640.09}{2108.0} = 0.9294$$

$$s_{19} = s_f + x_{19} s_{fg} = 1.8604 + (0.9294)(4.9603) = 6.4704 \text{ kJ/kg st-K.}$$

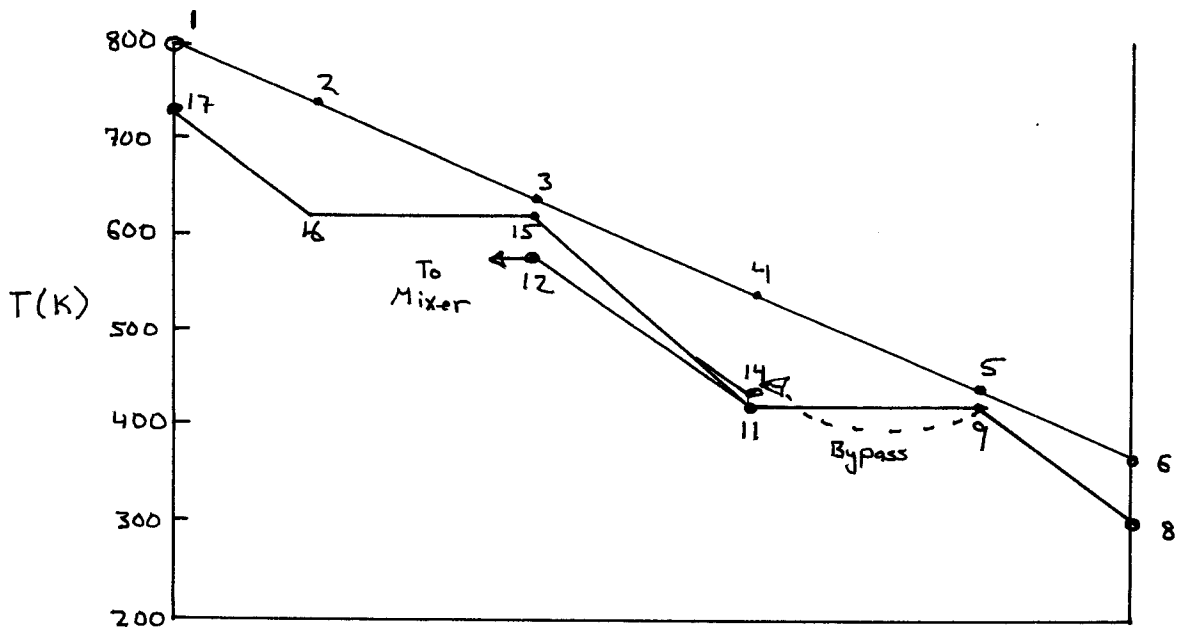
$$\textcircled{20} 5 \text{ kPa}, s_{20} = s_{19} \Rightarrow \text{mix: } x_{20} = \frac{s_{20} - s_f}{s_{fg}} = \frac{6.4704 - 0.4762}{7.9176} = 0.7571$$

20 Points

②

$$h_{20} = h_f + X_{20} h_{fg} = 137.75 + (0.7571)(2423.0) \frac{\text{KJ}}{\text{kg}} \Rightarrow h_{20} = 1972.15 \frac{\text{KJ}}{\text{kg}}$$

$$\begin{aligned} \dot{W}_T &= \dot{m}_{st, HP} (h_{17} - h_{18}) + \dot{m}_{st} (h_{19} - h_{20}) \\ &= \left[0.1131 \frac{\text{kg}}{\text{s}} \right] \left[3157.9 - 2460.25 \frac{\text{KJ}}{\text{kg}} \right] + \left[0.1469 \frac{\text{kg}}{\text{s}} \right] \left[2599.2 - 1972.15 \frac{\text{KJ}}{\text{kg}} \right] \\ &\Rightarrow \dot{W}_T = 171.02 \text{ KW} \end{aligned}$$



② Rankine: Capital cost: $\frac{600,000 \text{ KWe}}{\text{yr}} \mid \frac{1300 \$}{\text{KW}} = \$780. \text{E}+6$

Capital recovery factor: $\frac{A}{P} = \frac{i}{1 - (1+i)^{-n}} = \frac{0.05}{1 - (1+0.05)^{-30}} = 0.0651$

$\Rightarrow$ Annual cost of capital: $\frac{\$780. \text{E}+6}{0.0651} = 50,740,000 \$/\text{yr}$

Fuel cost: $\frac{600,000 \text{ KJ}_e}{\text{s}} \mid \frac{\text{KJ}_{Th}}{0.37 \text{ KJ}_e} \mid \frac{0.75}{1.055 \text{ KJ}} \mid \frac{\text{Btu}}{10^6 \text{ Btu}} \mid \frac{1.5 \$}{31.5 \text{E}+6 \$} = 54,470,000 \$/\text{yr}$

6 Points

Total annual cost: $\frac{50.74 + 54.47 \text{E}+6 \$/\text{yr}}{105.21 \text{E}+6 \$/\text{yr}} \Rightarrow \text{Unit cost} = 2.67 \$/\text{KW-hr}$

Combined: Capital cost: $\frac{400,000 \text{ KWe}}{\text{yr}} \mid \frac{\$550.}{\text{KW}} = \$220. \text{E}+6 \$/\text{yr}$

Annual cost of capital: $\frac{\$220. \text{E}+6 \$}{0.0651} = \$14.32 \text{E}+6 \$/\text{yr}$

Fuel cost: $\frac{400,000 \text{ KJ}_e}{\text{s}} \mid \frac{\text{KJ}_{Th}}{0.60 \text{ KJ}_e} \mid \frac{0.90}{1.055 \text{ KJ}} \mid \frac{\text{Btu}}{10^6 \text{ Btu}} \mid \frac{8 \$}{31.5 \text{E}+6 \$} = \$143,300,000/\text{yr}$

Total annual cost: $\frac{14.32 \text{E}+6 + 143.3 \text{E}+6 \$}{157.64 \text{E}+6 \$/\text{yr}} \Rightarrow \text{Unit cost} = 5.0 \$/\text{KW-hr}$

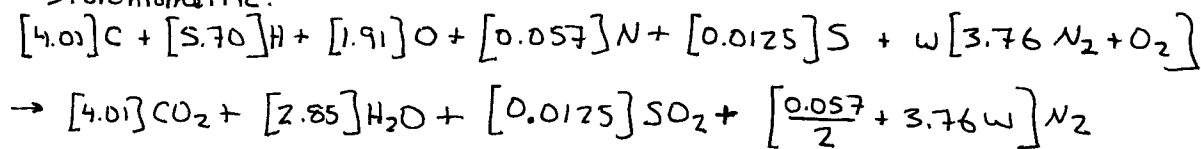
Investors hate uncertainty, especially for projects that have long payoff times such as power installations. For new coal-fired Rankine cycles, the main uncertainty has been the level to which new environmental regulations may force the addition of new expensive pollution control equipment during the plant's lifetime. For combined cycle systems, the uncertainty is the supply and cost of natural gas. The current cost of power from coal-fired Rankine is lower, even including advanced pollution control, which explains why you see action on site selection for new coal plants in the news these days (and the negative response from those communities near proposed plants). In general, investors are seeing less uncertainty when the cost of a coal plant, with best available pollution control technology, is less than natural gas systems fired on currently-priced gas.

③ Centralia coal analysis: (100 kg raw coal basis)

	% mass	kg	Kmoles
C	48.1	48.1	4.01
H	5.7	5.7	5.70
O	30.5	30.5	1.91
N	0.8	0.8	0.057
S	0.4	0.4	0.0125
ash	14.5	14.5	

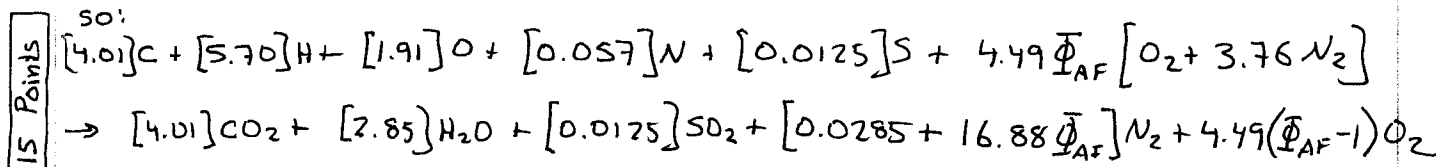
$$HHV = 4617.04 \frac{\text{Kcal}}{\text{kg}}$$

Stoichiometric:



O-atom balance: $1.91 + 2w = (2)(4.01) + 2.85 + (2)(0.0125)$
 $\Rightarrow w = 4.49$

so:



Next get h_f^0 for the coal. $\frac{4617.04 \text{ Kcal}}{\text{kg}} \mid \frac{4.184 \text{ KJ}}{\text{Kcal}} = 19,318 \frac{\text{KJ}}{\text{kg}} = HHV.$

Stoichiometric:

Species	Kmoles	h_f^0	$h - h_{298}$	
Coal	100 kg	$h_{f, \text{coal}}^0$	0	$H_R = h_{f, \text{coal}}^0$
O ₂	4.49	0	0	
N ₂	16.88	0	0	
CO ₂	4.01	-393,520	0	
H ₂ O	2.85	-285,830	0	$H_P = -2,396,341 \text{ KJ}/100 \text{ kg coal}$
SO ₂	0.0125	-296,840	0	
N ₂	0	0	0	

(4)

$$Q = H_P - H_R \Rightarrow -1,931,800 = -2,396,341 - h_{f, \text{coal}}^\circ \Rightarrow h_{f, \text{coal}}^\circ = -464,541 \frac{\text{kJ}}{\text{kg coal}}$$

for 100 kg coal

Now set up actual condition with $\Phi_{AF} = 1.20$

Species	Kmoles	h_f°	$h - h_{298}$	
Coal	100 kg	-464,591	0	} $H_R = -464,591 \frac{\text{kJ}}{100 \text{ kg coal}}$
O ₂	5.39	0	0	
N ₂	20.26	0	0	
CO ₂	4.01	-393,520	15,483 - 9364	} $H_P = -2,137,490 \frac{\text{kJ}}{100 \text{ kg coal}}$
H ₂ O	2.85	-241,820	15,080 - 9904	
SO ₂	0.0125	-296,840	6476 *	
N ₂	20.28	0	13,105 - 8669	
O ₂	0.90	0	13,228 - 8682	

$$* [h - h_{298}]_{\text{SO}_2} = C_{p, \text{SO}_2} (T - 298) = \left[42.60 \frac{\text{kJ}}{\text{kmole} \cdot \text{K}} \right] [450 - 298 \text{ K}] = 6476 \text{ kJ/kmole}$$

$$Q = H_P - H_R = -2,137,490 - (-464,591) \frac{\text{kJ}}{100 \text{ kg coal}}$$

$$\Rightarrow \boxed{Q = -1,672,898 \frac{\text{kJ}}{100 \text{ kg coal}}}$$

ME 430/599C – Advanced Energy
Problem Set 8 – Assigned November 3, Due November 9, 4:30pm

Note: The problem set is not quite as bad as it appears, as we are using information about the steam cycles developed in earlier problem sets. It still takes some work, however

The attached figure shows an oxyfuel IGCC system configured for CO₂ sequestration. Our goal is to get a rough idea of the efficiency of the cycle and the amount of CO₂ that needs to be recycled.

Air for the gasifier is at 298 K and is separated into O₂ and N₂ at 298 K, the O₂ stream being at 25 atm and the N₂ being at 1 atm. The coal has an ultimate analysis of 92.258% C, 7.742% H. (Assume no O, N, S, ash, or moisture. *Hint: use exact molecular weights.*) The HHV of the coal is 40 MJ/kg. This particular gasifier uses a dry powdered coal feed with no additional water (you can ignore the relatively small amount of work needed to compress the coal to the 25 atm gasifier pressure). The gasifier stoichiometry is selected such that the only products of the reaction are CO and H₂. The gasifier is adiabatic, and the products are cooled to 400 K by the gas cooler. The steam properties in the gas cooler Rankine cycle and the HRSG Rankine cycle can be assumed to be the same as those from Problem Set 6.¹ The combustor is adiabatic. The compressor and gas turbine can be assumed isentropic. The HRSG is assumed to operate such that the outlet is pure CO₂ mixed with liquid water, which is separated. Both are at 298 K. Oxygen is separated from air by a second, larger plant that discharges both streams at 298 K and 1 atm. The O₂ is directed to the compressor inlet, and the O₂ is stoichiometric relative to the fuel arriving from the gasifier. Enough CO₂ is redirected to the compressor inlet to provide a combustor outlet temperature of 1700 K.

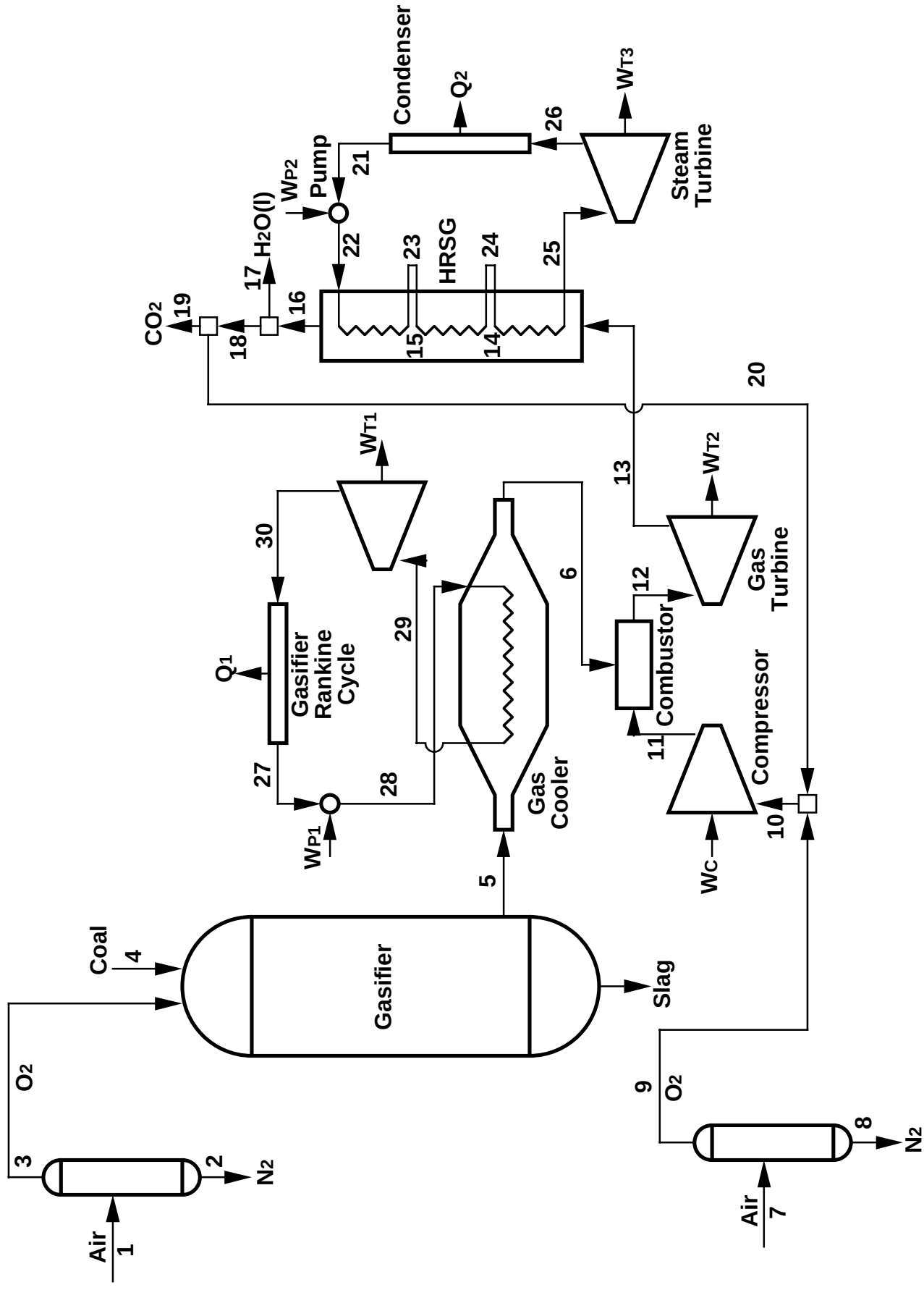
Finding the correct amount of CO₂ requires an iterative procedure in which the amount of CO₂ recycle is guessed, the outlet temperature of the compressor is calculated, and then this outlet temperature and the composition is used with the fuel gas in the equilibrium code to find an adiabatic combustor outlet temperature.

A new feature here is finding the isentropic outlet temperature for a compressor operating on a arbitrary gas mixture. The easiest way to do this is the constant Cp approach using the average Cp for the gas mixtures. An appropriate way to proceed is as follows:

- a) Estimate the outlet temperature of the compressor assuming the gas is pure CO₂. Note that this is a reasonable assumption as most of the gas will be CO₂. Use this to estimate approximately the average gas temperature in the compressor.
- b) Use this average temperature to get Cp and Cv for both O₂ and CO₂ (closest entry in the tables will do as this doesn't change much with temperature). Subsequent iterations will not change the outlet temperature enough to warrant changing the Cp and Cv values as you work forward.
- c) For your guessed value of n_{CO_2} , calculate the average Cp and Cv for the compressor gas. Use this to calculate the average value of Cp/Cv, and use this in the isentropic relations to find T_{11} .
- d) Take T_{11} and the oxidizer composition to the equilibrium code.

¹ Note that this allows you to work from the two Rankine cycles simply by calculating the ratio of $W_{\text{net}}/Q_{\text{in}}$, and then multiplying this by the respective Q's into these two cycles. No additional calculations are needed.

1. Assume 100 kg coal as a basis for your calculations. Find the enthalpy of formation of the coal on this basis (kJ/100 kg coal).
2. Find the amount of O_2 required by the gasifier (kmol).
3. Find the thermodynamic minimum amount of work required to perform the air separation (*i.e.*, work required by a reversible process that accepts air at 1 atm, 298 K and produces N_2 at 1 atm and O_2 at 25 atm, all at 298 K). Use as a basis 100 kg coal.
4. Assume the actual work required by the air separation is three times this. Compare this with the 1.3 MJ/kg O_2 figure from class. (This should be fairly close to the number given in class.)
5. Find the amount of heat extracted from the fuel gas in the gas cooler (kJ). *Hint:* This calculation is most easily approached by applying a first law to a *cv* that contains both the gasifier and the gas cooler. This avoids having to calculate the gasifier outlet temperature. Then find the net work from the gas cooler Rankine cycle (kJ). (Note that if you use the results of the prior problem set, this is a one-line calculation.)
6. Find the amount of O_2 required by the combustor (kmol), and the work required by the second air separation plant (kJ). Assume the second air separation plant has the same power requirement on a kmol O_2 basis as the first, even though the outlet O_2 pressures are different.
7. Use the equilibrium code to find the amount of CO_2 required by the compressor (kmol) and the work required by the compressor (kJ). *Hints:* As mentioned above, this will be a two step process. In the first, you will need to use your guess for CO_2 to find the outlet temperature of the compressor. In the second, you use the compressor outlet temperature and the composition in the equilibrium code to see if you are at 1700 K. Note that you should specify the stoichiometry as moles air/mole fuel or kg air/kg fuel to be sure you are getting the stoichiometry you intend.
8. Use the equilibrium code to find the exhaust temperature from the gas turbine. Find the net work from gas turbine cycle (kJ). (I got 1,310,516 kJ.)
9. Find the total heat rejected by the HRSG (kJ), and apply the Rankine efficiency to find the net work from the HRSG Rankine cycle (kJ).
10. Calculate the net work from the cycle (kJ) (including O_2 separation parasitic losses), and the net cycle efficiency based on the HHV of the 100 kg of coal. (I got a number between 44 and 48%.)



Element	Kg	MW (kg/kmole)	Kmols
C	92.258	12.011	7.68
H	7.742	1.008	7.68

Stoichiometric reaction with O_2 : $7.68C + 7.68H + wO_2 \rightarrow 7.68CO_2 + 3.84H_2O$
 $2w = [2][7.68] + [3.84] \Rightarrow w = 9.60$

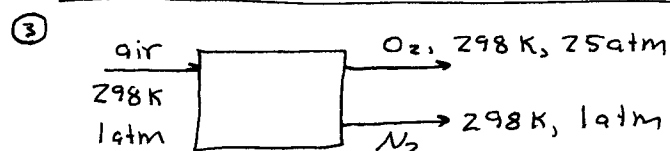
Species	Kmols	h_f°	
Coal	100 kg	$h_{f,coal}^\circ$	] $H_R = h_{f,coal}^\circ$
O_2	9.60	0	
CO_2	7.68	-393,520	] $H_P = -4,119,820 \text{ kJ/100 kg}$
H_2O	3.84	-285,830	

$$Q = -H_{HV} = -\frac{40 \text{ MJ}}{\text{kg}} \left| \frac{10^3 \text{ kJ}}{\text{MJ}} \right| \frac{100 \text{ kg}}{[100 \text{ kg}]} = -4,000,000 \text{ kJ/100 kg}$$

$$Q = H_P - H_R \Rightarrow -4,000,000 = -4,119,820 - h_{f,coal}^\circ$$

$$\Rightarrow h_{f,coal}^\circ = -119,820 \text{ kJ/100 kg}$$

② Gasifier reaction: $7.68C + 7.68H + qO_2 \rightarrow 7.68CO + 3.84H_2$
 $\Rightarrow q = 3.84 \Rightarrow O_2 = 3.84 \text{ kmols}$



$$W_{min} = \frac{h_{in} - h_{out}}{\text{all } T = 298} - T_0 (S_{in} - S_{out}) = -T_0 \left[n_{O_2} \left(-R \ln \frac{P_{O_2, in}}{P_{O_2, out}} \right) + n_{N_2} \left(-R \ln \frac{P_{N_2, in}}{P_{N_2, out}} \right) \right]$$

$$W_{min} = RT_0 \left[n_{O_2} \ln \left(\frac{P_{O_2, in}}{P_{O_2, out}} \right) + n_{N_2} \ln \left(\frac{P_{N_2, in}}{P_{N_2, out}} \right) \right]$$

$$\text{In } n_{O_2} = 3.84, \quad n_{N_2} = 3.76 n_{O_2} \Rightarrow 14.44$$

$$W_{min} = \left(8.314 \frac{\text{kJ}}{\text{kmol} \cdot \text{K}} \right) (298 \text{ K}) \left[(3.84 \text{ kmols}) \ln \left[\frac{0.21}{25} \right] + (14.44 \text{ kmols}) \ln \left[\frac{.79}{1} \right] \right]$$

$$W_{min} = -53,905 \text{ kJ}$$

④

$$W_q = 3W_{min} = \frac{3 \left| \begin{array}{c|c|c|c} 53,905 \text{ kJ} & 100 \text{ kg Coal} & \text{kmol } O_2 & \text{MJ} \\ \hline 100 \text{ kg coal} & 3.84 \text{ kmols } O_2 & 32 \text{ kg } O_2 & 10^3 \text{ kJ} \end{array} \right|}{10^3 \text{ kJ}}$$

$$[3] \left[53,905 \frac{\text{kJ}}{100 \text{ kg coal}} \right] \Rightarrow W_q = 161,715 \frac{\text{kJ}}{100 \text{ kg coal}} \Rightarrow W_q = 1.316 \text{ MJ/kg } O_2$$

⑤

Species	Kmols	h_f°	$h - h_{298}$	
Coal	100 kg	-119,820	0	] $H_R = -119,820$
O_2	3.84	0	0	
CO	7.68	-110,530	11,644 - 8669	] $H_P = -814,664$
H_2	3.84	0	11,426 - 8468	

$$Q = H_P - H_R = -814,664 - (-119,820) \Rightarrow Q = -694,844 \text{ kJ}$$

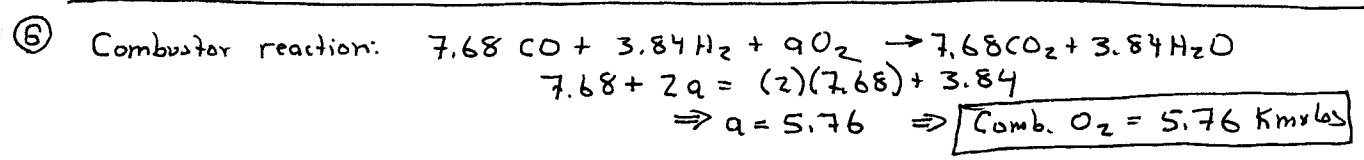
⑤ From Problem Set 6: $Q_R = \dot{m}_a (h_5 - h_8) = \frac{1.0204 \text{ kg mix}}{\text{kg air}} \frac{-474.95 - (-966.87) \text{ kJ}}{\text{kg mix}}$

$Q_R = \frac{501.95}{\text{kg air}} \text{ kJ/kg air}$

$\eta_R = \frac{W_R}{Q_R} = \frac{172.19}{501.95} = \underline{\underline{0.343}}$

Using this in our present cycle:

$W_{R, \text{Gas}} = 0.343 Q_R$
 $= [0.343] [-694,844 \text{ kJ}]$
 $\Rightarrow \boxed{W_{R, \text{Gas}} = 238,358. \text{ kJ}}$



5.76 kmol O ₂	32 kg	1.316 MJ	10 ³ kJ
	kmol	kg	kJ

$\Rightarrow \boxed{W_{O_2} = 242,565. \text{ kJ}}$

⑦ First, assume all the gas is CO₂ $\Rightarrow T_{11} = T_{10} (r_p)^{k-1/k} \Rightarrow T_{11} = 298 (25)^{1.289/1.289}$
 to get an estimate for $\bar{T}$ in compressor. $\Rightarrow T_{11} = 613.25 \text{ K}$
 So the average T in compressor is $\frac{613.25 + 298}{2} = 455 \text{ K} \approx 450 \text{ K}$.

We will use 450 K as the $\bar{T}$ for our C_p & C_v

@ 450 K:

	CO ₂	O ₂
C_p	43.03	30.59
C_v	34.76	22.27

So $\bar{C}_p = \frac{n_{\text{CO}_2} C_{p, \text{CO}_2} + n_{\text{O}_2} C_{p, \text{O}_2}}{n_{\text{CO}_2} + n_{\text{O}_2}} = \frac{43.03 n_{\text{CO}_2} + (30.59)(5.76)}{n_{\text{CO}_2} + 5.76}$

$\bar{C}_p = \frac{43.03 n_{\text{CO}_2} + 176.20}{n_{\text{CO}_2} + 5.76}$

$\bar{C}_v = \frac{n_{\text{CO}_2} C_{v, \text{CO}_2} + n_{\text{O}_2} C_{v, \text{O}_2}}{n_{\text{CO}_2} + n_{\text{O}_2}} = \frac{34.76 n_{\text{CO}_2} + (22.27)(5.76)}{n_{\text{CO}_2} + 5.76}$

$\bar{C}_v = \frac{34.76 n_{\text{CO}_2} + 128.27}{n_{\text{CO}_2} + 5.76}$

$\bar{k} = \bar{C}_p / \bar{C}_v$

$T_{11} = T_{10} r_p^{\bar{k}-1/\bar{k}} = (298)(25)^{\bar{k}-1/\bar{k}}$

In the code we need to enter fuel relative moles:

"air" ~~not~~ relative moles

CO = 2
H ₂ = 1
O ₂ = 5.76
CO ₂ = n_{CO_2}

Enter stoichiometry as $\frac{\text{moles air}}{\text{mole fuel}} = \frac{5.76 + n_{\text{CO}_2}}{7.68 + 3.84} = \boxed{\frac{5.76 + n_{\text{CO}_2}}{11.52}}$

Pressure = 25 atm, $T_{\text{fuel}} = 298 \text{ K}$, Problem Type = HP

- Procedure:
- Guess n_{CO_2}
 - Calc. T_{11}
 - Adjust oxidant ~~stoichiometry~~ relative moles, air/fuel ratio, T_{11}
 - run code
 - Iterate on n_{CO_2} until $T_{02} = 1700 \text{ K}$,

A spreadsheet was then assembled that calculated all the boxed quantities on the previous page. The code was then run:

$$\left. \begin{array}{l} \text{Fuel: } \begin{array}{l} \text{CO} = 2 \\ \text{H}_2 = 1 \end{array} \\ \text{Ox: } \begin{array}{l} \text{O}_2 = 5.76 \\ \text{CO}_2 = n_{\text{CO}_2} \end{array} \end{array} \right| \begin{array}{l} \text{moles air} \\ \text{mole fuel} \\ \text{from eqn} \end{array} \left| \text{HP} \right| \left. \begin{array}{l} T_{\text{fuel}} = 298 \\ T_{\text{Ox}} = \text{from eqn} \\ P = 25 \text{ atm} \end{array} \right\} \begin{array}{l} \text{Iterate on } n_{\text{CO}_2} \text{ until:} \\ T_{12} = 1700 \text{ K} \end{array}$$

n_{CO_2}	C_p	C_v	k	T_{11}	moles air/ mole fuel	T_{12} from code
20	40.2484472	31.9670031	1.25906226	577.9014	2.23611111	2233.26
40	41.4641608	33.1877185	1.24938268	566.567543	3.97222222	1658.15
38.54	41.4125553	33.1359007	1.24977908	567.030701	3.84548611	1687.62
37.93	41.3899725	33.113225	1.24995293	567.233863	3.79253472	1700.4

$$\Rightarrow S_{12} = 6.4709 \text{ kJ/kg mix-K}, \quad h_{12} = -7366.319 \text{ kJ/kg}$$

$$\Rightarrow n_{\text{CO}_2} = 37.93 \text{ kmol}$$

$$W_c = n_c \bar{c}_p (T_{11} - T_{10}) = (37.93 + 5.76 \text{ kmol}) (41.39 \frac{\text{kJ}}{\text{kmol-K}}) (567.2 - 298 \text{ K})$$

$$\Rightarrow W_c = 486,802 \text{ kJ}$$

⑧ Run code ~~to~~ with $P = 1 \text{ atm}$ to get $S_{13} = S_{12}$

$$\left. \begin{array}{l} \text{Fuel} \\ \text{Ox} \end{array} \right\} \begin{array}{l} \text{as above} \\ \text{as above} \end{array} \left| \begin{array}{l} \text{moles air} \\ \text{mole fuel} \end{array} = 3.79 \right| \text{TP} \left| \begin{array}{l} P = 1 \text{ atm} \\ T_f = \text{guess} \end{array} \right\} \uparrow$$

$$\begin{array}{c} T(\text{K}) \\ 1000 \\ 1100 \end{array} \quad \begin{array}{c} S(\text{kJ/kg mix-K}) \\ 6.3975 \\ 6.5196 \end{array}$$

$$T_{13} = 1060.1 \text{ K}$$

$$6.4719 \quad \Rightarrow h_{13} = -8232.079 \text{ kJ/kg mix}$$

$$\text{Mass products: } \sum n_i M_{W_i} = (7.68)(28) + (3.84)(2) + (5.76)(32) + (37.93)(44) = 2076 \text{ kg mix / 100 kg coal}$$

$$W_T = h_{12} - h_{13} = \frac{-7366.319 - (-8232.079) \text{ kJ}}{\text{kg mix} \mid 100 \text{ kg coal}} = 2076 \text{ kJ/kg mix}$$

$$\Rightarrow W_T = 1,797,318 \text{ kJ}$$

$$W_{\text{net,GT}} = W_T - W_c = 1,797,318 - 486,802$$

$$\Rightarrow W_{\text{net,GT}} = 1,310,516 \text{ kJ}$$

⑨

$$h_{16} = n_{\text{CO}_2} h_{f,\text{CO}_2}^\circ + n_{\text{H}_2\text{O}} h_{f,\text{H}_2\text{O}}^\circ$$

$$= (37.93 + 7.68)(-393,520) + (3.84)(-285,830) =$$

$$h_{13} = \frac{-8232.079 \text{ kJ}}{\text{kg mix} \mid 100 \text{ kg coal}} = \frac{-17,089,796 \text{ kJ}}{100 \text{ kg coal}}$$

$$Q_R = h_{13} - h_{16} = -17,089,796 - (-19,046,034) \frac{\text{kJ}}{100 \text{ kg coal}} \Rightarrow$$

$$Q_{R,2} = 1,956,238 \frac{\text{kJ}}{100 \text{ kg coal}}$$

$$W_{R,2} = \eta_R Q_R = (0.343)(1,956,238 \frac{\text{kJ}}{100 \text{ kg coal}})$$

$$\Rightarrow W_{R,2} = 682,284 \frac{\text{kJ}}{100 \text{ kg coal}}$$

$$(10) W_{\text{net}} = W_B + W_{R1} + W_{R2} = W_{O_{2,1}} - W_{O_{2,2}}$$

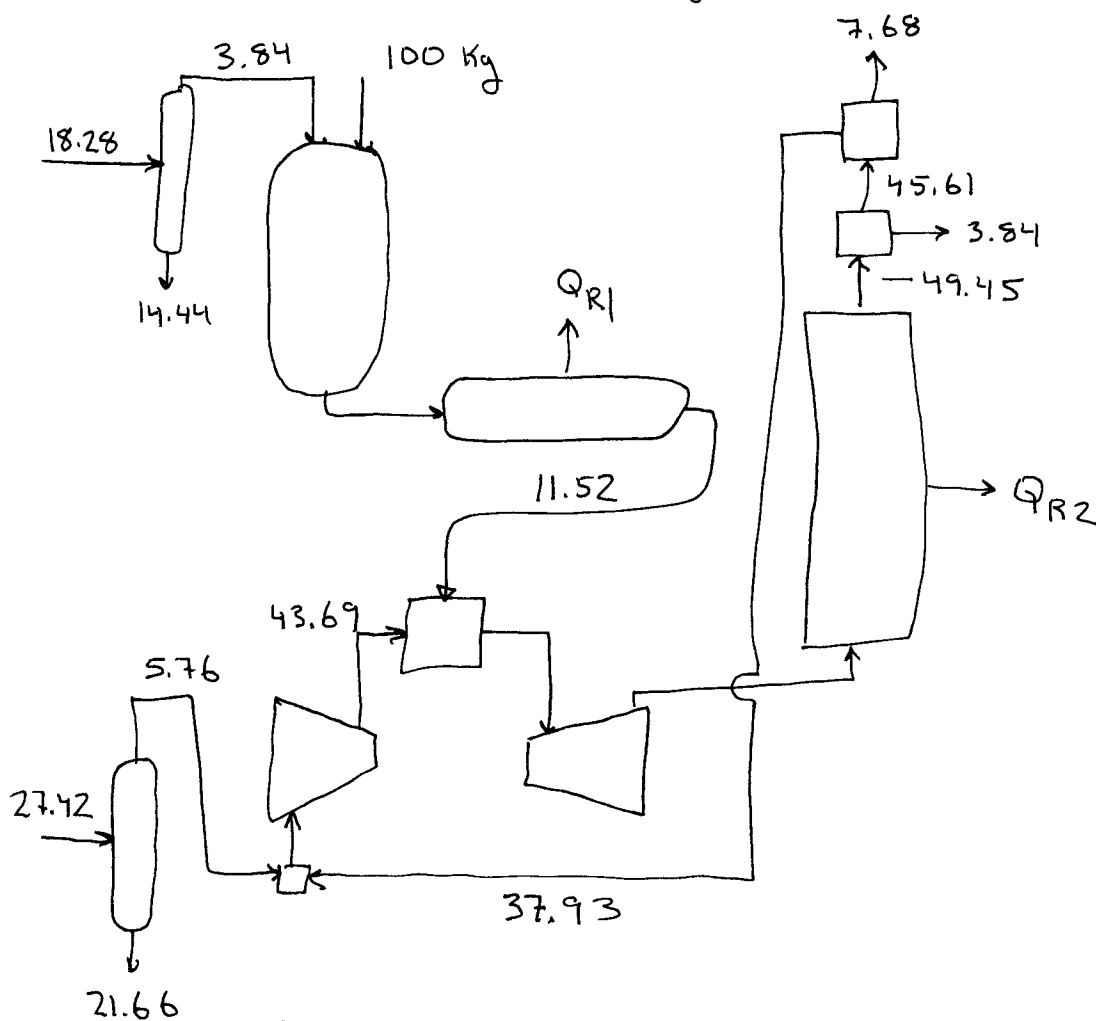
$$= 1,310,516 + 238,358 + 682,284 - 161,715 - 242,565 \frac{\text{kJ}}{100 \text{ kg coal}}$$

$$\Rightarrow W_{\text{net}} = 1,826,878 \frac{\text{kJ}}{100 \text{ kg coal}}$$

$$\eta_{\text{cycle}} = \frac{W_{\text{net}}}{\text{Coal HHV}} = \frac{1,826,878 \text{ kJ}}{100 \text{ kg coal}} \bigg| \frac{\text{kg}}{40,000 \text{ kJ}}$$

$$\Rightarrow \eta_{\text{cycle}} = 0.4567$$

So the plant looks like the following (molar flows)



Our calculation η_{cycle} is somewhat high due to $\eta_c = \eta_T = 1$ for the gas turbine cycle. Note the huge amount of CO_2 recycle needed

ME 430/599C – Advanced Energy
Problem Set 9 – Assigned November 10, Due November 16, 4:30pm

1. A piece of ceramic contains 1 milligram of U-238 as a component in the surface glaze. The U-238 undergoes decay via the release of an alpha particle. Use half-life data to estimate the number of alpha particles per second that are released by the ceramic.
2. A nuclear battery is fueled by Sr-90. If the thermoelectric generator associated with the battery has an efficiency of 5%, find the initial mass of Sr-90 needed to provide an electric power output of 100 Watts 10 years after the battery is built.
3. A fission reaction between a neutron and U-235 yields Rb-86 as one of the products and two neutrons.
 - (a) Find the final stable products of the reaction. For the isotopes that list more than one decay product, keep track of how much material goes down each path. You may ignore decay paths that are less than 1%, and you may ignore decays other than alpha and beta.
 - (b) Find the total energy release (MEV) associated with the original fission reaction and the subsequent decay to stable products.
4. The Columbia Generating Station at Hanford is the only operating nuclear power plant in the Pacific Northwest. It's net power output is 1100 MW_e, while the net mechanical power output of the Rankine cycle is 1250 MW. The condenser cooling water is provided by six forced draft evaporative coolers (similar to those in the UW power plant). As such, you don't see the huge towers that are normally associated with natural draft cooling systems. The missing power is used elsewhere in the plant, including the power for pumping and especially the fans in the evaporative coolers, and generator and other electrical losses. The plant sells it's electricity to BPA at cost, which in 2005 is quoted as being 3.34¢/kW-hr.

The system is a boiling water reactor, with a GE Type-5 core. This system operates at 7 MPa boiler pressure and no superheat. Assume the system operates on a simple Rankine cycle with a condenser pressure of 7.5 kPa and a steam turbine efficiency of 90%.

- (a) Find the Rankine cycle efficiency ($W_{\text{net}}/Q_{\text{in}}$).
- (b) Find the steam flow rate (kg/s).
- (c) Assuming an average energy release of 200 MEV/fission, find the mass of uranium ore (expressed as kg of elemental uranium) that must be mined each year to fuel this reactor. Note that the mined uranium includes both U-235 and U-238, and what I want is the combined mass of these two isotopes that must be mined.
- (d) If the fuel is enriched to 5% U-235, find the total mass of UO₂ that must be provided each year (includes both U-235 and U-238).
- (e) Assuming the cooling water enters the condenser at 20°C and leaves at 28°C, find the flow rate of cooling water needed.
- (f) Assuming the cooling water is returned to 20°C by evaporation in the cooling towers, use enthalpy of vaporization data to roughly estimate how much water is lost by evaporation. This must be made up from river water, so this number is important as it sets the plant's external water requirement.
- (g) A typical value for neutron flux in the core of boiling water reactors is 1.8E+18 neutrons/m²-s. Use this, along with fission cross-section data to estimate the kmols of U-235 that must be present in the core to provide the plant's thermal power generation. (*Hint: This is a real-world problem in the sense that you have all the tools you need, but I haven't told you how to approach the problem. Many of the problems you will run into in the outside world will be like this, so think it through.*)

$$\textcircled{1} \quad {}_{92}^{238}\text{U} \rightarrow {}_2^4\alpha + {}_{90}^{234}\text{Th} \quad t_{1/2} = 4.468 \text{E}+9 \text{ yr}$$

$$\frac{n}{n_i} = \exp\left[-\frac{t}{\tau^*}\right] \Rightarrow 0.5 = \exp\left[-\frac{4.468 \text{E}+9 \text{ yr}}{\tau^*}\right] \Rightarrow \tau^* = 6.45 \text{E}+9 \text{ yr}$$

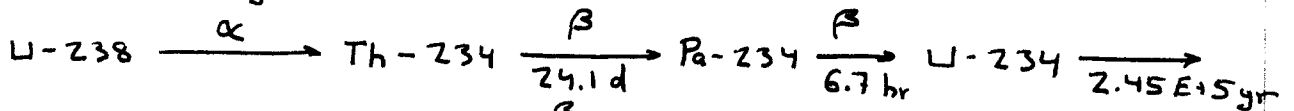
$$\frac{dn}{dt} = -\frac{n_i}{\tau^*} \exp\left[-\frac{t}{\tau^*}\right] ; \text{ now } \Rightarrow t=0 \Rightarrow \frac{dn}{dt} = -\frac{n_i}{\tau^*}$$

$$\frac{dn}{dt} = \frac{1 \text{ mg}}{10^6 \text{ mg}} \left| \frac{\text{Kg}}{238 \text{ Kg}} \right| \left| \frac{\text{K mole}}{6.023 \text{E}+26 \text{ atoms}} \right| \left| \frac{\text{yr}}{31.5 \text{E}+6 \text{ s}} \right|$$

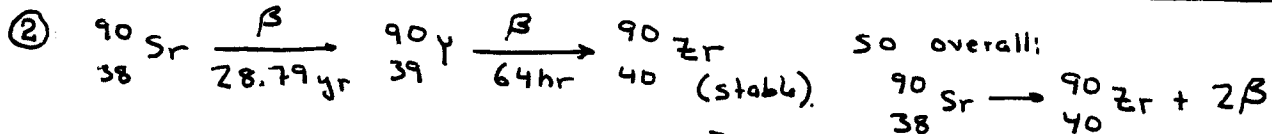
$$\Rightarrow \frac{dn}{dt} = 12.5 \frac{\text{decays}}{\text{s}}$$

5 Points

Note that the decay path is:



This means you would also see $25 \beta/\text{s}$. Note that subsequent decay of U-234 would be insignificant if initial sample was free of U-234.



$$\left. \begin{array}{l} m_R = 89.9077376 \text{ AMU} \\ m_P = 89.9047073 + 2[0.000549] \end{array} \right\} \Rightarrow \Delta m = 0.00194 \text{ AMU}$$

$$\frac{0.00194 \text{ AMU}}{\text{decay}} \left| \frac{1.49 \text{E}-10 \text{ J}}{\text{AMU}} \right| = 2.88 \text{E}-13 \text{ J/decay.}$$

$$\frac{n}{n_i} = \exp\left[-\frac{t}{\tau^*}\right] \Rightarrow 0.5 = \exp\left[-\frac{28.79}{\tau^*}\right] \Rightarrow \tau^* = 41.54 \text{ yr}$$

$$\frac{dn}{dt} = \frac{n_i}{\tau^*} \exp\left[-\frac{t}{\tau^*}\right] \Rightarrow \text{power} = \left[\frac{\text{energy}}{\text{decay}} \right] \frac{n_i}{\tau^*} \exp\left[-\frac{t}{\tau^*}\right]$$

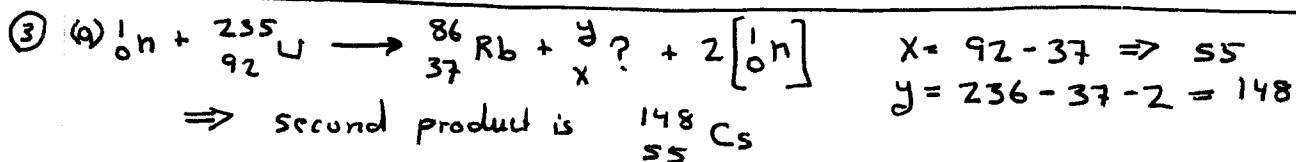
5 Points

$$\text{Heat needed} = \frac{100 \text{ J/s}}{0.05} = 2000 \text{ J/s}$$

$$2000 \frac{\text{J}}{\text{s}} = \frac{2.88 \text{E}-13 \text{ J}}{\text{decay}} \left| \frac{n_i}{41.54 \text{ yr}} \right| \left| \frac{\text{yr}}{31.5 \text{E}+6 \text{ s}} \right| \exp\left[-\frac{10 \text{ yr}}{41.54 \text{ yr}}\right]$$

$$\Rightarrow n_i = 1.156 \text{E}+25 \text{ atoms}$$

$$\frac{1.156 \text{E}+25 \text{ atoms}}{6.023 \text{E}+26 \text{ atoms}} \left| \frac{\text{K mole}}{90 \text{ Kg}} \right| \Rightarrow m_i = 1.73 \text{ Kg}$$

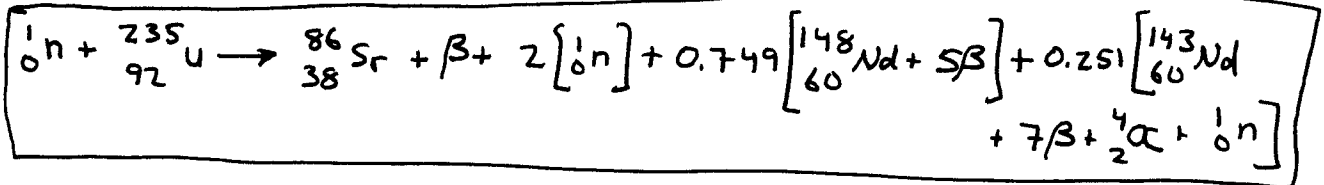


$$\begin{array}{c}
 \begin{array}{ccccccc}
 {}^{148}_{55}\text{Cs} & \xrightarrow[\text{74.9\%}]{\beta, 140\text{ ms}} & {}^{148}_{56}\text{Ba} & \xrightarrow[0.6075]{\beta} & {}^{148}_{57}\text{La} & \xrightarrow[1.428\text{s}]{\beta} & {}^{148}_{58}\text{Ce} & \xrightarrow[563]{\beta} & {}^{148}_{59}\text{Pr} \\
 & & & & & & & & \downarrow \beta \text{ 2.27 m} \\
 & & & & & & & & {}^{148}_{60}\text{Nd (stable)}
 \end{array} \\
 \\
 \begin{array}{ccccccc}
 {}^{148}_{55}\text{Cs} & \xrightarrow[\text{25.1\%}]{\beta + \text{on}} & {}^{147}_{56}\text{Ba} & \xrightarrow[0.8935]{\beta} & {}^{147}_{57}\text{La} & \xrightarrow[4.0155]{\beta} & {}^{147}_{58}\text{Ce} & \xrightarrow[56.45]{\beta} & {}^{147}_{59}\text{Pr} \\
 & & & & & & & & \downarrow \beta \text{ 13.4 m} \\
 & & & & & & & & {}^{147}_{60}\text{Nd} \xrightarrow[10.98\text{d}]{\beta} {}^{147}_{61}\text{Pm} \xrightarrow[2.6234\text{yr}]{\beta} {}^{147}_{62}\text{Sm} \xrightarrow[1.06\text{E}+11\text{yr}]{\alpha} {}^{143}_{60}\text{Nd (stable)}
 \end{array}
 \end{array}$$

The other decay reaction is:

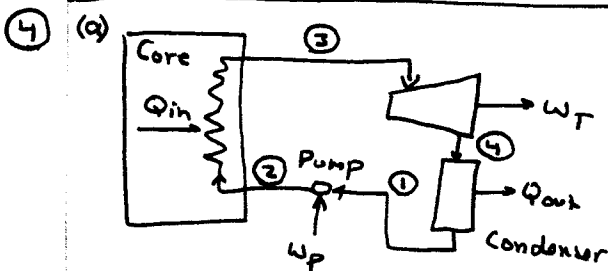
$${}_{37}^{86}\text{Rb} \xrightarrow[18.63\text{ d}]{\beta} {}_{38}^{86}\text{Sr}_{(\text{stable})}$$

5 Points



(b) Reactants: ${}^1_0\text{n}$ 1.008665
 ${}^{235}_{92}\text{U}$ 235.0439
 Products: ${}^{2.251}_{86}\text{Kr}$ 2.251 [1.008665]
 ${}^{0.749}_{38}\text{Sr}$ 0.749 [1.008665]
 ${}^{0.251}_{143}\text{Xe}$ 0.251 [1.008665]
 ${}^{5.50}_{143}\text{Xe}$ 5.5 [1.008665]
 ${}^{0.251}_{143}\text{Xe}$ 0.251 [1.008665]

$m_R = 236.052565 \text{ AMU}$
 $m_P = 235.848194 \text{ AMU}$
 $\Rightarrow \Delta m = 0.204371 \text{ AMU}$



① Sat. Liq. 7.5 kPa $\Rightarrow$
 $h_1 = 168.79 \text{ kJ/kg}$
 $v_1 = 1.008 \text{ E-3 m}^3/\text{kg}$
 $T_1 = 40.29^\circ\text{C}$

$$\textcircled{2} \quad w_p = \frac{V_1(P_2 - P_1)}{k_g} = \frac{1.008 \text{E-}3 \text{ m}^3}{1} \frac{7000 - 7.5 \text{ kPa}}{1} = 7.05 \frac{\text{N}}{\text{kg}}$$

③ 7000 kPa, Sat. Vapor $\Rightarrow h_3 = 2772.1 \text{ kJ/kg}$, $s_3 = 5.8133 \text{ kJ/kg-K}$.

④ $S_4 = S_3$, $P_4 = 7.5 \text{ KPa} \Rightarrow S_{\text{at. mix.}}$

$$X_4 = \frac{S_4 - S_f}{S_{1q}} = \frac{5.8133 - 0.5764}{7.6750} = 0.6823$$

$$h_{4,s} = h_f + X_{4,s} h_{fg} = 168.79 + [0.6823][2406] = 1810.49 \text{ kJ/kg}$$

$$\eta_r = \frac{w_a}{w_s} = \frac{h_3 - h_4}{h_3 - h_{4,s}} \Rightarrow 0.90 = \frac{2772.1 - h_4}{2772.1 - 1810.49} \Rightarrow h_4 = 1906.64 \text{ kJ/kg}$$

$$\eta_{\text{cycle}} = \frac{W_{\text{net}}}{Q_{\text{in}}} = \frac{h_3 - h_4 - w_p}{h_3 - h_2} = \frac{2772.1 - 1906.64 - 7.05}{2772.1 - 175.84} \Rightarrow \eta_{\text{cycle}} = 33.06\%$$

(b) $W_{\text{net}} = 2772.1 - 1906.64 - 7.05 = 858.41 \text{ kJ/kg}$

$$\frac{12,500,000 \text{ kJ}}{\text{s}} = \dot{m}_{\text{st}} \cdot \left[858.41 \frac{\text{kJ}}{\text{kg}_{\text{st}}} \right] \Rightarrow \dot{m}_{\text{st}} = 14,566.18 \text{ kg/s}$$

(c) $Q_{\text{in}} = \frac{W_{\text{net}}}{\eta_{\text{cycle}}} = \frac{12,500,000 \text{ kJ/s}}{0.3306} = 3.77 \times 10^7 \text{ kJ/s}$

$$\frac{3.77 \times 10^7 \text{ kJ}}{\text{yr}} \times \frac{\text{fission}}{200 \text{ MEV}} \times \frac{\text{MEV}}{1.60 \times 10^{-16} \text{ J}} = 3.72 \times 10^{27} \text{ atoms of U-235 consumed/yr.}$$

$3.72 \times 10^{27} \text{ atoms U-235}$ yr	atoms U	Kmole	238 kg U
	$0.0072 \text{ atoms U-235}$	$6.023 \times 10^{26} \text{ atoms}$	Kmole U

$$\Rightarrow \text{Raw uranium} = 204,267 \text{ kg as element}$$

(d) $\frac{3.72 \times 10^{27} \text{ atoms U-235}}{\text{yr}} \times \frac{\text{atom U}}{0.05 \text{ atom U-235}} \times \frac{\text{Kmole U}}{6.023 \times 10^{26} \text{ atoms U}} \times \frac{270 \text{ kg UO}_2}{\text{Kmole U}}$

$$\Rightarrow \text{Fuel mass} = 33,352 \frac{\text{kg UO}_2}{\text{yr}}$$

(e) $\dot{Q}_{\text{out}} = \dot{m}_{\text{st}} (h_4 - h_1) = (14,566.18 \frac{\text{kg}}{\text{s}}) (1906.64 - 168.79 \text{ kJ/kg}) = 2,530,600 \frac{\text{kJ}}{\text{s}}$

Cooling water: $\dot{Q}_{\text{out}} = \dot{m}_w C_{p,w} (\Delta T)$
 $2,530,600 \text{ kJ/s} = \dot{m}_w (4.184 \frac{\text{kJ}}{\text{kg} \cdot \text{K}}) (8^\circ\text{C}) \Rightarrow \dot{m}_w = 76,604 \frac{\text{kg}}{\text{s}}$

(f) $\dot{Q}_{\text{out}} = \dot{m}_{\text{evap}} h_{\text{fg}} \Rightarrow 2,530,600 \frac{\text{kJ}}{\text{s}} = \dot{m}_{\text{evap}} (2454.1 \frac{\text{kJ}}{\text{kg}})$
 $\Rightarrow \dot{m}_{\text{evap}} = 1,031 \frac{\text{kg}}{\text{s}}$

15 Points

(g) From notes, $\frac{\text{fissions}}{\text{m}^2 \cdot \text{s}} = \sigma_f \Phi_n N_u$

From above we have $\frac{3.72 \times 10^{27} \text{ fissions}}{\text{yr}} \times \frac{\text{yr}}{3.16 \times 10^7 \text{ s}} = 1.17 \times 10^{20} \frac{\text{fissions}}{\text{s}}$

Multiply both sides of our equation by reactor volume:

$$\frac{\text{fissions}}{\text{s}} = \sigma_f \Phi_n N_u \quad \text{where } N_u = \text{total } \text{atoms of U-235 in core}$$

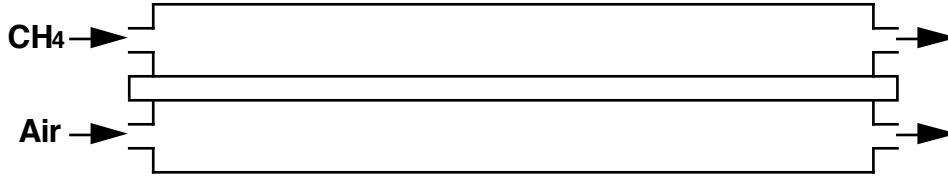
$$N_u = \left[\frac{\text{fission}}{\text{s}} \right] \left[\frac{1}{\sigma_f \Phi_n} \right] = \frac{1.17 \times 10^{20} \text{ fissions/s}}{584.5 \times 10^{-28} \text{ m}^2 \times 1.8 \times 10^{18} \text{ n}} = 6.023 \times 10^{26} \text{ atoms}$$

$$N_u = 1.85 \times 10^6 \text{ Kmole U-235}$$

Note that we consume $6.18 \text{ Kmole U-235/yr}$. This means that between fuelings we will have more poisons and will need to control Φ_n via control rods to a lower level.

ME 430/599C – Advanced Energy
Problem Set 10 – Assigned November 26, Due December 3, 4:30pm

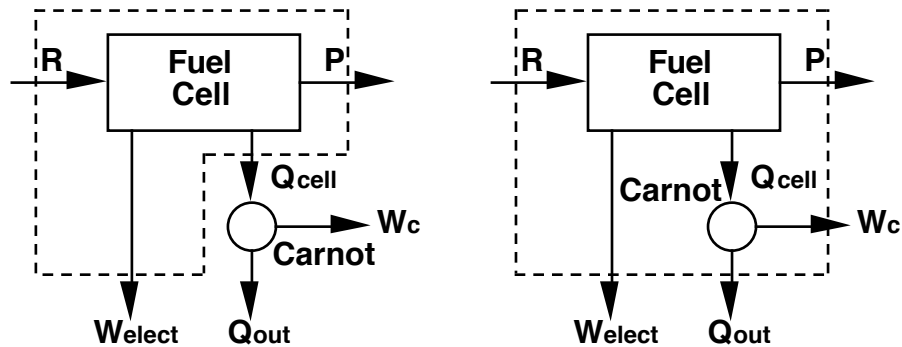
1. A hypothetical fuel cell burns CH_4 and air. The ion transported across the electrolyte is O^{2-} . Assume the cell operates at 1000 K (inlet gases, cell, and products are all at this temperature). The total pressure is 1 atm. throughout.



- (a) Find the mole fractions and partial pressures of each component at the point where half the CH_4 has been reacted.
 (b) The $W_{\max}$ term that goes into the Nernst equation is our usual:

$$W_{\max} = h_R - h_P - T(s_R - s_P)$$

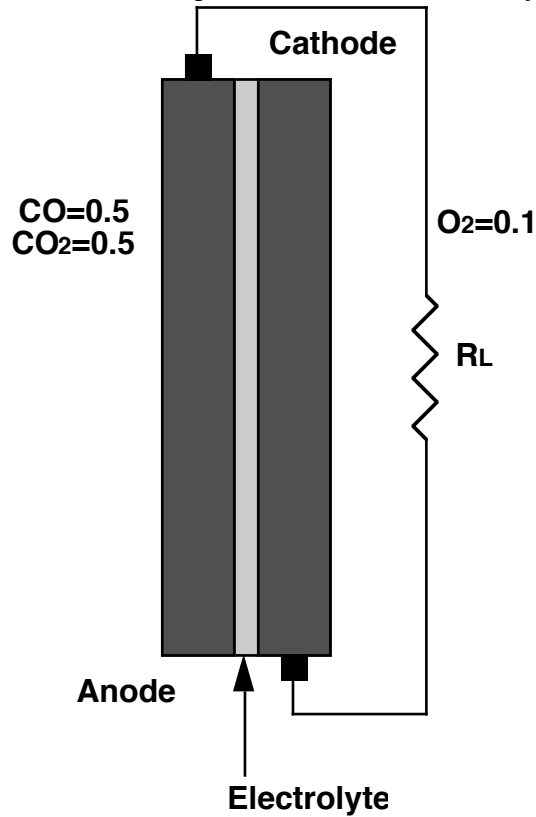
Should the T in this equation be 298 K or 1000 K? Use the following figures to help you decide (dashed lines are possible cv boundaries).

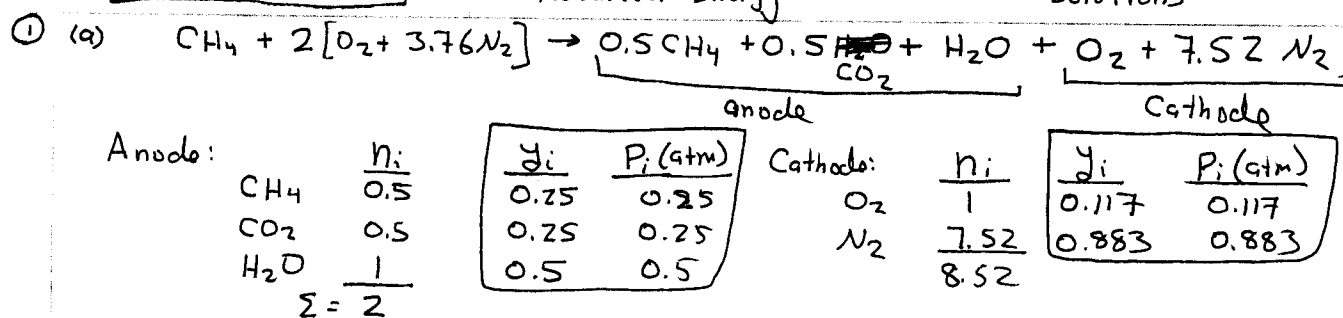


- (c) Find the theoretical cell voltage.
2. A fuel cell is fueled by CO and air. Oxygen ions (O^{2-}) are the species that conduct through the electrolyte. At a certain point in the cell, the anode gas contains equimolar CO and CO_2 . On the cathode, the oxygen is at 0.1 mole fraction with the rest being N_2 . The total pressure is 1 atm everywhere. At this point, the theoretical cell potential is 0.9653 volts.

The cell consists of a 10 cm by 10 cm square of electrolyte that is 1 mm thick operated at 1000 K. The porous anode and cathode sandwich the electrolyte, and are each 5 mm thick. The electrochemical reactions occur at the electrode/electrolyte interface. The effective resistances of the anode and cathode to current flow (between the reaction sites and the terminals) is $0.0025 \, \Omega$ in each. The resistivity of the electrolyte to oxygen ions is $1.0\text{E-}3 \, \Omega\text{-m}$, and the resistivity to electron flow is $1.0 \, \Omega\text{-m}$. The flow of charge in the electrolyte can be assumed to be one-dimensional. The activation overpotential parameters are: exchange current density, $i_0=50 \text{ amps/m}^2$, and $\alpha=0.5$. We will ignore concentration overpotential effects. Use this information to generate a plot of load current versus load voltage between the open-circuit and short-circuit conditions. Although this calculation is best approached

using a program like Excel, do a hand calculation, showing all your steps, for the case of $R_L = 0.005 \, \Omega$. *Hint:* This process will require some iteration since the cell voltage is influenced by the activation overpotential, which is a function of the cell current. Appropriate use of Excel, with cut and paste, can be used to easily approach this problem.



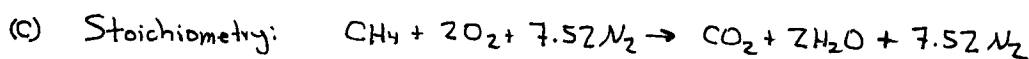


(b) Voltage represents fuel cell w_{max} normalized by the amount of charge moved (rather than kmols reactants as usual).

First configuration: The CV produces w_{elect} and q crossing the boundary at 1000 K. Since the TDS term is based on the q leaving the cell, the appropriate T is 1000 K here.

Second configuration: The CV produces w_{elect} plus work from the heat being delivered to 298 K. The w_{carnot} is not generated by the cell, but rather by a separate bottoming cycle that is included in the CV. Since the q leaves at 298 K, this is the appropriate T here.

Since the voltage is based on w_{elect} only, it would be incorrect to include w_{carnot} , and the correct answer is $T = 1000 \text{ K}$.
If $T = 298 \text{ K}$ then w_{max} includes the carnot work.



Species	Kmols	h_f°	$h - h_{298}$	$S_{f,i}$	$P_i (\text{atm})$	S_i
CH_4	1	-74,850	38,528	252.60	0.25	264.13
O_2	2	0	31,389 - 8682	243.471	0.117	261.31
N_2	7.52	0	30,129 - 8669	228.057	0.883	229.09
CO_2	1	-393,520	42,769 - 9364	269.215	0.25	280.74
H_2O	2	-241,820	35,882 - 9904	232.597	0.50	238.36
N_2	7.52	0	30,129 - 8669	228.057	0.883	229.09

Methane: $dh = C_p dT \Rightarrow h_{1000} - h_{298} = \int_{298}^{1000} C_p dT$

(more approximate, but good)

C_p is often represented as a polynomial curve-fit of T . This can be directly substituted into the equation and integrated. An easier approach is to evaluate C_p at the average $T = \frac{298+1000}{2} = \sim 650 \text{ K}$, and then treat C_p as constant.

$$h_{1000} - h_{298} = \bar{C}_p (1000 - 298)$$

$$C_p \left(\frac{\text{kJ}}{\text{kmol} \cdot \text{K}} \right) = 19.89 + 5.024 \times 10^{-2} T + 1.269 \times 10^{-5} T^2 - 11.01 \times 10^{-9} T^3$$

@ 650 K, $C_p = 54.88 \text{ kJ/kmol} \cdot \text{K}$

$$h_{1000} - h_{298} = [54.88 \text{ kJ/kmol} \cdot \text{K}] [1000 - 298 \text{ K}] = 38,528 \text{ kJ/kmole}$$

$$ds^\circ = \frac{C_p}{T} dT \quad S_{1000}^\circ - S_{298}^\circ = \int_{298}^{1000} \frac{C_p}{T} dT = C_p \ln \left[\frac{1000}{298} \right] = [54.88 \frac{\text{kJ}}{\text{kmol} \cdot \text{K}}] \ln \left[\frac{1000}{298} \right] = 66.44 \text{ kJ/kmol} \cdot \text{K}$$

②

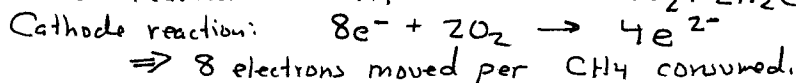
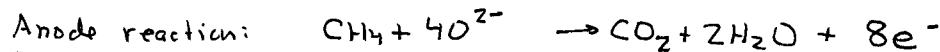
$$S_{1000}^{\circ} = S_{298}^{\circ} + (S_{1000}^{\circ} - S_{298}^{\circ}) = 186.16 + 66.44 \text{ KJ/Kmole} \cdot \text{K} = 252.60 \text{ KJ/Kmole} \cdot \text{K}$$

$$\Rightarrow H_R = +170,471 \text{ KJ/Kmole CH}_4 \quad H_P = -630,420 \text{ KJ/Kmole CH}_4$$

$$S_R = 2509.51 \text{ KJ/Kmole CH}_4 \cdot \text{K} \quad S_P = 2480.22 \text{ KJ/Kmole CH}_4 \cdot \text{K}$$

$$W_{\max} = H_R - H_P - T(S_R - S_P) = 170,471 - (-630,420) - (1000)(2509.51 - 2480.22)$$

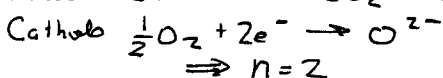
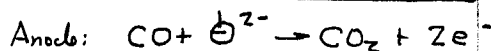
$$W_{\max} = 771,598 \text{ KJ/Kmole CH}_4$$



$$V = \frac{771,598 \text{ KJ}}{\text{Kmole CH}_4} \left| \frac{\text{Kmole CH}_4}{8 \text{ Kmole e}^-} \right| \left| \frac{\text{Kmole e}^-}{9.64 \text{ E}+7 \text{ coul}} \right| \left| \frac{10^3 \text{ J}}{\text{KJ}} \right| \Rightarrow \boxed{E^{\circ} = 1.0005 \text{ Volts}}$$

② First get electrolyte resistances:

$$R = \frac{\sigma \delta}{A c}$$



$$R_{e,i} = \frac{1.0 \text{ } \Omega \cdot \text{m}}{100 \text{ cm}^2} \left| \frac{10^{-3} \text{ m}}{\text{m}^2} \right| = 1.0 \text{ E}-4 \text{ } \Omega$$

$$R_{e,e} \Rightarrow 1.0 \text{ } \Omega \cdot \text{m} \Rightarrow R_{e,e} = 0.1 \text{ } \Omega$$

Next, equivalent R for circuit:

$$R = R_{e,i} + \frac{1}{\frac{1}{R_{e,e}} + \frac{1}{R_a + R_c + R_L}} = 1.0 \text{ E}-4 + \frac{1}{\frac{1}{0.1} + \frac{1}{0.0025 + 0.0025 + 0.005}}$$

$$\Rightarrow R = 0.009191 \text{ } \Omega$$

$$i_{\text{cell}} = \frac{E^{\circ} - V_{\text{act}}}{R} = \frac{0.9653 - 0}{0.009191} = 105.03 \text{ A} \quad [\text{for first iteration, let } V_{\text{act}} = 0]$$

$$i_{\text{cell}} = \frac{105.03 \text{ A}}{\text{cm}^2} \left| \frac{10^4 \text{ cm}^2}{\text{m}^2} \right| = 10,030 \text{ A/m}^2$$

$$V_{\text{act}} = \frac{RT}{\alpha n F} \ln \left[\frac{i}{i_0} \right] = \frac{8.314 \text{ KJ}}{\text{Kmole} \cdot \text{K}} \left| \frac{1000 \text{ K}}{0.5} \right| \left| \frac{\text{Kmole e}^-}{2} \right| \left| \frac{10^3 \text{ J}}{9.64 \text{ E}+7 \text{ coul}} \right| \left| \frac{1}{\text{Kg}} \right| \ln \left[\frac{10,030}{50} \right]$$

$$= 0.0862 \text{ V} \Rightarrow V_{\text{act}} = 0.457 \text{ V}$$

Now repeat

$$i_{\text{cell}} = \frac{0.9653 - 0.457}{0.009191} = 55.30 \text{ A}, \quad V_{\text{act}} = (0.0862 \text{ V}) \ln \frac{5530}{50} = 0.406 \text{ V}$$

$$\text{Again } i_{\text{cell}} = \frac{0.9653 - 0.406}{0.009191} = 60.85 \text{ A}, \quad V_{\text{act}} = (0.0862 \text{ V}) \ln \frac{6085}{50} = 0.414 \text{ V}$$

$$\text{Again } i_{\text{cell}} = 59.97 \text{ A}, \quad V_{\text{act}} = 0.413 \text{ V} \quad \checkmark \text{ OK}$$

$$\text{Now get } i_{\text{leak}} = \frac{E_0 - V_{\text{act}} - i_{\text{cell}} R_{e,i}}{R_{e,e}} = \frac{0.9653 - 0.413 - (59.97)(1.0 \text{ E}-4)}{0.1} = 5.46 \text{ A}$$

$$i_L = i_{\text{cell}} - i_{\text{leak}} = 59.97 - 5.46 \Rightarrow \boxed{i_L = 54.51 \text{ A}}$$

$$V_L = R_L i_L = [0.005 \text{ } \Omega] [54.51 \text{ A}] \Rightarrow \boxed{V_L = 0.272 \text{ V}}$$

12 Points

ME 430/599C – Advanced Energy
Problem Set 11/Final Project – Assigned December 4, Due December 13, 4:30PM

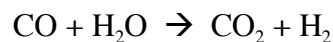
The attached figure shows the basic steam reforming process that is used for most of the H_2 manufactured in this country. Methane (298 K, 2.6 MPa) is mixed with steam (300°C, 2.6 MPa), with a molar ratio of 2.93 moles water vapor per mole methane. The mixture is introduced into tubes packed with nickel catalyst. The reforming reaction is endothermic, so an auxiliary flame provides the needed heat around the outside of the tubes. The reaction occurs at 1050 K, and the reformer gas exits at that temperature. The gas at that point is in thermochemical equilibrium and it contains only CO , CO_2 , H_2O , H_2 , and CH_4 as major species. This is cooled and passed through water gas shift catalysts to convert all the CO to CO_2 and some of the H_2O to H_2 . The gas is finally cooled to 298 K and all the water is condensed out. It then passes through a pressure-swing absorption system that separates the H_2 into one stream and the CO_2 and remaining CH_4 into the other. The latter is fed back to the reformer flame to recover the fuel value of the CH_4 .

The flame used in the reformer is methane/air, 20% excess air, with all reactants at 298 K. This gas exits the reformer at 1100 K, and is then cooled to 298 K in a steam generator (H_2O out is a vapor).

All the cooling required in the process is done by raising steam. Feedwater at 20°C and 2.6 MPa is available. Enough steam is raised to provide all the steam needed by the reformer as well as additional steam that can be exported from the process. (Often these plants are located within petroleum refineries, where the steam can be used in another process. Alternately, one could use the steam in a Rankine cycle or for heating.)

Our goal is to understand the mass and energy flows and losses associated with the steam reforming process. For this calculation, use as a basis one kmole CH_4 **entering the reformer** (note that since additional CH_4 is needed by the heater, the total consumption of CH_4 will be more than one kmole).

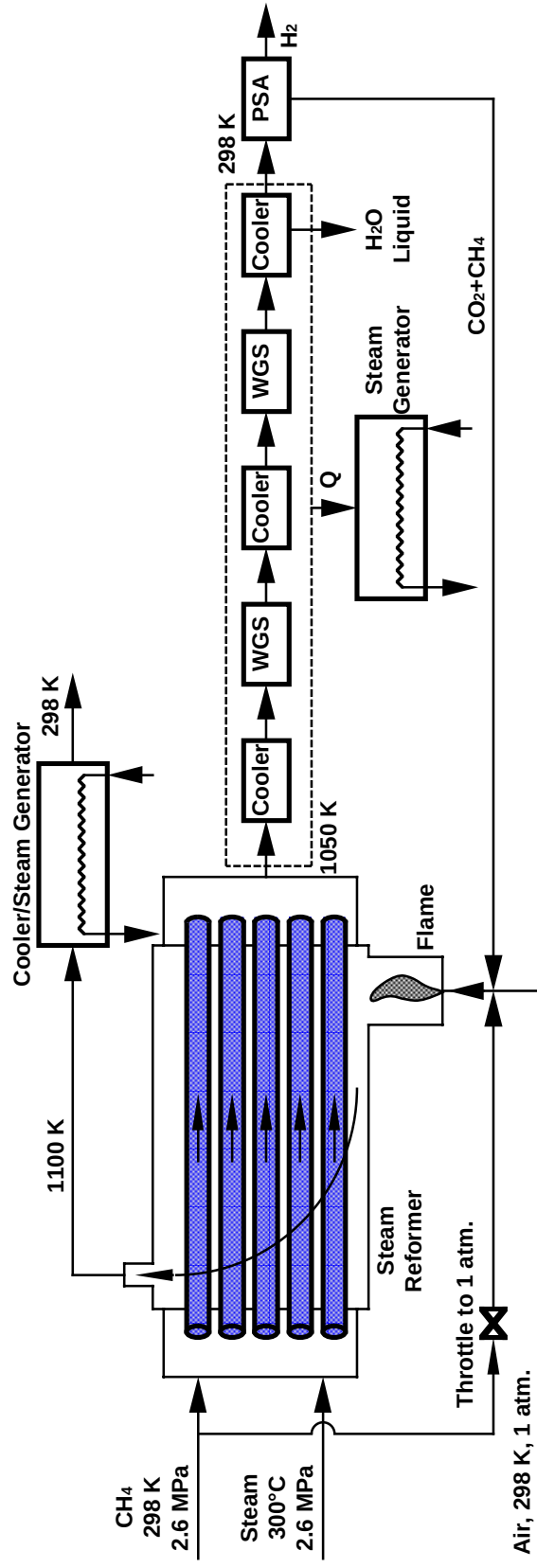
1. Make use of the equilibrium code to find the composition of the product gas leaving the reformer, and the amount of heat needed by the reformer. Express the composition as a table including the kmoles of each species. (*Hints:* In the code, make the fuel CH_4 , and the oxidant H_2O . Note that when doing the enthalpy balance on the reformer, get the inlet steam h from the ideal gas tables, not the steam tables. Although this is not exactly correct, using the ideal gas table will keep the calculation on the same $h=0$ reference point, while using the steam table requires a careful adjustment of the steam table zero point.)
2. Assume all the coolers and water-gas shift reactors can be lumped into a single CV as shown in the figure. These reactors act to convert all of the remaining CO to CO_2 via

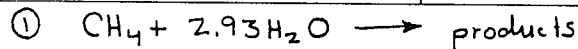


The reactors do not touch the remaining CH_4 (do not run the equilibrium code to get the outlet condition). Also, the last cooler condenses all the remaining water out as liquid.

Using these assumptions, find the final product composition entering the PSA (table of kmols) and the amount of heat extracted from the lumped CV.

3. The heat to the reformer is supplied by burning CH_4 . Assume the flame is fueled by CH_4 and 20% excess air. The combustion gas leaves the reformer at 1100 K. Find the kmols of CH_4 required by the flame. (As an aside, note that a good countercurrent flow design could get the outlet temperature below 1050 K, with a resulting reduction in the amount of CH_4 required.)
4. A portion of the CH_4 needed by the flame is available from the PSA. Subtract the PSA contribution from the total needed by the flame to get the actual amount of CH_4 needed from the feedstock line. You may ignore the effect on the flame of the CO_2 in the PSA offgas.
5. Find the amount of heat removed from the 1100 K combustion product gas stream.
6. Assuming all heat extracted is used to raise steam (from feedwater at 20°C and 2.6 MPa to 300°C, 2.6 MPa), find the total kg of steam raised (use the steam table here!).
7. Subtract the steam needed by the process to get the total amount of steam that is available for export from the process.
8. Calculate the raw efficiency for the process by the ratio of the LHV of the CH_4 required against the LHV of the H_2 produced. I got 67.3%



Get inlet h

	Kmoles	h_f°	$h - h_{298}$	$n_i (h_f^\circ + h - h_{298})$
CH_4	1	-74,850	0	-74,850
H_2O	2.93	-241,820	19,426 - 9904	-680,633

This is original w. CH_4 in reformer exhaust. See pp. 3-4 for rework with reformer exhaust CH_4 -free

$$h = -755,483.$$

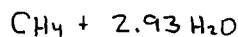
Run code:

$$\left. \begin{array}{l} \text{Fuel: } \text{CH}_4 \\ \text{Ox: } \text{H}_2\text{O} \end{array} \right| \begin{array}{l} \text{moles} \\ \text{O}_2/\text{mole fuel} \end{array} = \left. \begin{array}{l} \text{TP} \\ T = 1050 \text{ K} \end{array} \right| P = 2600 \text{ kPa} \left\{ h = -7727.611 \text{ kJ/kg mix} \right.$$

Species	mole fraction	Kmoles
H_2	0.4184	2.156
H_2O	0.3876	1.998
CO	0.0566	0.292
CO_2	0.06215	0.320
CH_4	0.07527	0.388

Note that since inlet $C=1$, $n_{\text{CO}} + n_{\text{CO}_2} + n_{\text{CH}_4} = 1$

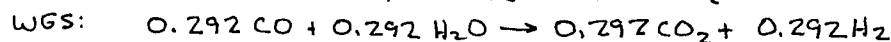
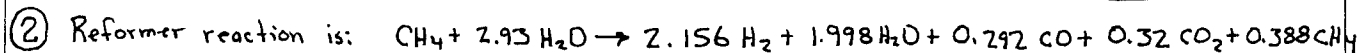
$$\Rightarrow \frac{1}{0.0566 + 0.06215 + 0.07527} = 5.154$$

 $\Rightarrow$ mult all mole fractions by this to get Kmoles
 $\Rightarrow$ note that H and O atoms balance also check.

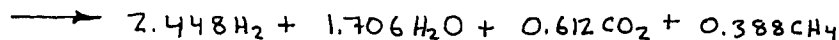
$$16 + (2.93)(18) = 68.74 \text{ kg}$$

$$h_{\text{out}} = \frac{-7727.611 \text{ kJ}}{\text{kg mix}} \left| \frac{68.74 \text{ kg mix}}{\text{kmole CH}_4} \right| = -531,196 \frac{\text{kJ}}{\text{kmole}}$$

$$q = h_{\text{out}} - h_{\text{in}} = -531,196 - [-755,483] \Rightarrow q = 224,287 \text{ kJ/kmole CH}_4$$

So subtract 0.292 from CO , H_2O & add 0.292 to CO_2 , H_2

WGS products

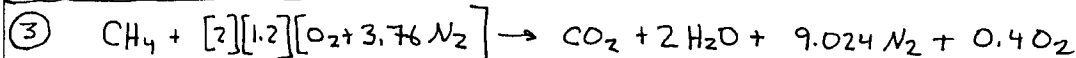
Now get h for this, treating H_2O as liquid.

	Kmoles	h_f°	$h - h_{298}$	$n_i (h_f^\circ + h - h_{298})$
H_2	2.448	0	0	0
H_2O	1.706	-285,830	0	-487,626
CO_2	0.612	-393,520	0	-240,834
CH_4	0.388	-74,850	0	-29,082

$$h_{\text{out}} = -757,542 \text{ kJ/kmole}$$

$$q = h_{\text{out}} - h_{\text{in}} = -757,542 - [-531,196] \Rightarrow q = -226,346 \text{ kJ/kmole}$$

Species	Kmoles
H_2	2.448
CO_2	0.612
CH_4	0.388

 $\Leftarrow$ Into PSA.Since $T < 1200 \text{ K}$, this composition is fine.

	Kmoles	h_f°	$h - h_{298}$	$n_i (h_f^\circ + h - h_{298})$
CH_4	1	-74,850	0	-74,850
O_2	2.4	0	0	0
N_2	9.024	0	0	0
CO_2	1	-393,520	48,258 - 9364	-354,626
H_2O	2	-241,820	40,071 - 9904	-423,306
N_2	9.024	0	33,426 - 8669	223,407
O_2	0.4	0	34,899 - 8682	10,487

$$h_R = -74,850$$

$$h_P = -544,038$$

$$q_{comb} = h_P - h_R = -544,038 - [-74,850] = -469,188 \frac{\text{KJ}}{\text{Kmol combust CH}_4}$$

$$\text{so: } \frac{224,287 \text{ KJ}}{\text{Kmol reformer CH}_4} \bigg| \frac{\text{Kmol comb CH}_4}{469,188 \text{ KJ}} \Rightarrow \frac{\text{Combust CH}_4}{\text{Reformer CH}_4} = 0.478$$

$$\text{Combust CH}_4 = 0.478 \text{ Kmols}$$

$$④ \quad 0.478 - 0.388 \Rightarrow \text{CH}_4 \text{ from inlet line to combustor} = 0.09 \text{ Kmols}$$

$$⑤ \quad \begin{array}{c|c|c|c|c} & \text{Kmols} & h_f^\circ & h - h_{298} & h_i (h_f^\circ + h - h_{298}) \\ \hline \text{CO}_2 & 1 & -393,520 & 0 & -393,520 \\ \text{H}_2\text{O} & 2 & -241,820 & 0 & -483,640 \\ \text{N}_2 & 9.024 & 0 & 0 & 0 \\ \text{O}_2 & 0.4 & 0 & 0 & 0 \end{array} \quad \left. \vphantom{\begin{array}{c|c|c|c|c} & \text{Kmols} & h_f^\circ & h - h_{298} & h_i (h_f^\circ + h - h_{298}) \end{array}} \right\} h = -877,160 \frac{\text{KJ}}{\text{Kmol CH}_4 \text{ (comb)}}$$

$$q = h_{out} - h_{in} = -877,160 - [-544,038] = -333,122 \text{ KJ/Kmol combust CH}_4$$

$$\frac{333,122 \text{ KJ}}{\text{comb CH}_4} \bigg| \frac{0.478 \text{ comb CH}_4}{\text{Reformer CH}_4} \Rightarrow q = -159,232 \frac{\text{KJ}}{\text{Kmol Ref CH}_4}$$

$$⑥ \quad \begin{array}{l} \text{Steam: } 20^\circ\text{C, } 2.6 \text{ MPa} \Rightarrow h_{in} = 83.915 \text{ KJ/kg} \\ \quad \quad \quad 300^\circ\text{C, } 2.6 \text{ MPa} \Rightarrow h_{out} = 2757.64 \text{ KJ/kg} \quad 3002.7 \text{ KJ/kg} \\ q = 2757.64 - 83.915 = 2673.72 \text{ KJ/kg steam.} \\ \quad \quad \quad 2918.8 \end{array}$$

$$\text{Total } q \text{ to steam: } 226,346 + 159,232 = 385,578 \text{ KJ/Kmol CH}_4$$

$$\text{Steam Generated: } \frac{385,578 \text{ KJ}}{\text{Kmol CH}_4} \bigg| \frac{\text{Kg Steam}}{2673.72 \text{ KJ}} \Rightarrow M_{st} = 143.94 \text{ Kg} \quad \boxed{132.1}$$

$$⑦ \quad \text{Steam needed: } \frac{2.93 \text{ Kmols}}{\text{Kmol}} \bigg| \frac{18 \text{ Kg}}{\text{Kmol}} = 52.47 \text{ Kg} \quad \boxed{79.6}$$

$$\text{Export steam: } 143.94 - 52.47 \Rightarrow M_{st} (\text{export}) = 91.20 \text{ Kg}$$

$$⑧ \quad \text{Methane in: } \frac{1 + 0.09 \text{ Kmols}}{\text{Kmol CH}_4} \bigg| \frac{800,800 \text{ KJ}}{\text{Kmol CH}_4} = 872,872 \text{ KJ}$$

$$\text{Hydrogen out } \frac{2.448 \text{ Kmols}}{\text{Kmol H}_2} \bigg| \frac{240,000 \text{ KJ}}{\text{Kmol H}_2} = 587,520 \text{ KJ}$$

$$\eta = \frac{587,520}{872,872} \Rightarrow \eta = 67.31\%$$

Redo of PS #11 w/o CH₄ in Reformer Outlet

- ① • Reactant composition and h unchanged:
• Code setup unchanged

Code Output:

Species	mole fraction	Kmoles
H ₂	0.566	3.356
H ₂ O	0.2653	1.573
CO	0.1085	0.643
CO ₂	0.06014	0.357

Note that since $C=1$,

$$n_{CO} + n_{CO_2} = 1$$

$\Rightarrow$ Scaling factor for mole fractions is:

$$\frac{1}{0.1085 + 0.06014} = 5.930$$

Also: $h_p = -6469.896 \text{ kJ/kg mix}$

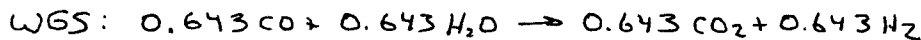
From original reactants weigh 68.74 kg

$$\Rightarrow h_p = \frac{-6469.896 \text{ kJ}}{\text{kg mix}} \left| \frac{68.74 \text{ kg mix}}{\text{kmole CH}_4} \right| = -444,741 \text{ kJ/kmole CH}_4$$

$$g = h_p - h_R = -444,741 - (-755,483) \text{ kJ/kmole}$$

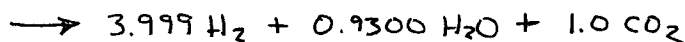
$$\Rightarrow g = 310,742 \text{ kJ/kmole CH}_4$$

- ② Reformer reaction is: $\text{CH}_4 + 2.93 \text{ H}_2\text{O} \rightarrow 3.356 \text{ H}_2 + 1.573 \text{ H}_2\text{O} + 0.643 \text{ CO} + 0.357 \text{ CO}_2$



So subtract 0.643 from CO, H₂O, and add 0.643 to H₂ and CO₂.

WGS Products:



Now get h for this, treating H₂O as liquid-

Species	Kmoles	h_f	$h - h_{298}$	$h_i (h_f^o + h - h_{298})$
H ₂	3.999	0	0	0
H ₂ O	0.93	-285,830	0	-265,822
CO ₂	1.0	-393,520	0	-393,520

$$h_p = -659,342 \text{ kJ/kmole}$$

$$g_{\text{WGS}} = h_p - h_R = -659,342 - (-444,741) \text{ kJ/kmole}$$

$$\Rightarrow g_{\text{WGS}} = -214,601 \text{ kJ/kmole CH}_4$$

Into PSA:	Species	Kmoles
	H ₂	3.999
	CO ₂	0.93

- ③ Problem 3 is unchanged up through the value of

$$g_{\text{comb}} = -469,188 \text{ kJ/kmole comb CH}_4$$

$$\text{so: } \frac{310,742 \text{ kJ}}{\text{kmole reformer CH}_4} \left| \frac{\text{kmole comb CH}_4}{469,188 \text{ kJ}} \right| \Rightarrow \frac{\text{comb CH}_4}{\text{Ref CH}_4} = 0.662$$

$$\Rightarrow \text{Comb CH}_4 = 0.662 \text{ kmole}$$

④ All CH_4 to combustor must be externally supplied.

⑤ This stays the same through $q = -333,122 \text{ kJ/kmole Combust CH}_4$

$$\frac{333,122 \text{ kJ}}{\text{kmole Comb CH}_4} \bigg| \frac{0.662 \text{ kmols Comb CH}_4}{1 \text{ kmole Ref CH}_4} \Rightarrow q = -220,527 \frac{\text{kJ}}{\text{kmole Ref CH}_4}$$

⑥ This stays the same through $q = 2918.8 \text{ kJ/kg steam}$.

$$\text{Total } q \text{ to steam} = 214,601 + 220,527 \Rightarrow = 435,128 \text{ kJ/kmol Ref CH}_4$$

$$\text{Steam generated} = \frac{435,128 \text{ kJ}}{\text{kmole Ref CH}_4} \bigg| \frac{\text{kg Steam}}{2918.8 \text{ kJ}} \Rightarrow \boxed{\dot{m}_{\text{st}} = 149.08 \text{ kg}}$$

⑦ Steam needed by reformer = $2.93 \text{ kmols} = 52.47 \text{ kg}$.

$$\Rightarrow \text{Export steam} = 149.08 - 52.47 \Rightarrow \boxed{m_{\text{st}}(\text{export}) = 96.61 \text{ kg}}$$

⑧ Methane in = $\frac{1 + 0.662 \text{ kmols}}{1 \text{ kmole}} \bigg| \frac{800,800 \text{ kJ}}{\text{kmole}} = 1,330,930 \text{ kJ}$

$$\text{Hydrogen out} = \frac{3.999 \text{ kmols}}{1 \text{ kmole}} \bigg| \frac{240,000 \text{ kJ}}{\text{kmole}} = 960,000 \text{ kJ}$$

$$\eta = \frac{960,000}{1,330,930} \Rightarrow \boxed{\eta = 72.13\%}$$

ME 430/529 – Advanced Energy Systems
Learning Objectives – Midterm Exam No. 1

Prior to the first exam (Tuesday, October 24, 2017), you should be able to:

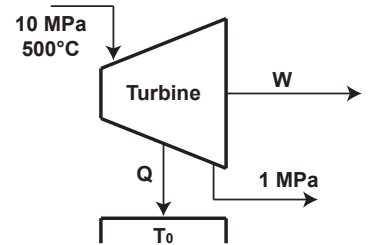
1. Perform standard Rankine and Brayton cycle calculations, insofar as they are used in combined cycle systems.
2. Evaluate the availability of resource streams to do work (*e.g.*, high-temperature and/or high pressure air or steam flows). You should be able to use these to find the efficiency with which the availability is utilized in a real process to generate power.
3. Evaluate the availability of reacting systems to do work.
4. Use stoichiometric calculations to find stoichiometry given product gas composition, or find the product gas composition given the stoichiometry.
5. Use first law balances around reacting systems to find heat losses, adiabatic flame temperatures, or required reactant preheat temperatures.
6. Perform performance calculations on combined cycle systems, including being able to identify whether a pinch-point violation is occurring within a HRSG.

The exam will be open book and open notes, but no computers (be sure to bring your thermo book for access to property tables, and a calculator). The time limit is 55 minutes. Obviously, a 55 minute exam will not permit any kind of detailed analysis such as we have done on the homework. Also, we will not be able to cover every item listed above. You should instead expect shorter calculation problems that focus on specific parts of larger problems. Your goal should be to understand the principles associated with Items 1-6 in a way that allows you to apply these principles to new problems that may not look exactly like the homework you have done. I suggest you study the homework solutions carefully if you have had any problems with the homework. Although the test is open book, if you need to do extensive reading of book or notes during the exam, or you attempt to follow a book/handout example, you will probably have a time problem.

ME 430/529 – Advanced Energy
Example Midterm Exam 1

For all problems, $T_0=298\text{ K}$ and $P_0=1.0\text{ atm}$.

- 1.(25%) For the non-adiabatic steam turbine shown at right, $w=300\text{ kJ/kg}$, the heat loss to the environment is $q=23.5\text{ kJ/kg}$. Find the irreversibility of the turbine, including the heat transfer process (kJ/kg).



- 2.(25%) Find the availability of saturated liquid R-134a at 600 kPa (kJ/kg). You may assume the dead state is 20°C and 100 kPa for this problem.

- 3.(25%) The combustor at right accepts 1 kmole of H_2 and y kmoles of O_2 (both as separate streams at 298 K and 1.0 atm), reacting them to produce products consisting of H_2O and O_2 at 1200 K. Find the value of y .



- 4.(25%) For Problem 3, assume $y=5$ and find the reversible work connecting the reactants and the products (kJ/kmole H_2).

① In: 298 K, 1 atm $\Rightarrow h_{in} = 298.18 \text{ kJ/kg}$, $P_{r,i} = 1.3543$

Opt: 600 K, $\Rightarrow h_{out} = 607.2 \text{ kJ/kg}$

$P_{r,2} = P_{r,i}$, $r_p = [1.3543][7.6871] = 10.37 \Rightarrow h_{out,s} = 533.98 \text{ kJ/kg}$

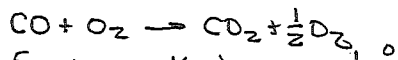
$\eta_c = \frac{W_s}{W_a} = \frac{h_{out,s} - h_{in}}{h_{out} - h_{in}} = \frac{533.98 - 298.18}{607.2 - 298.18} \Rightarrow \boxed{\eta_c = 76.31\%}$

②

$W_{max} = h_i - h_o - T_o(S_i - S_o)$. Sat. Liq, 1000 kPa $\Rightarrow h_o = 107.32 \text{ kJ/kg}$, $S_i = 0.39189 \text{ kJ/kg-K}$
Dead state: 20°C, 100 kPa $\Rightarrow h_o = 272.17 \text{ kJ/kg}$, $S_o = 1.0918 \text{ kJ/kg-K}$.

$W_{max} = 107.32 - 272.17 - (293)(0.39189 - 1.0918) \Rightarrow W_{max} = 40.22 \text{ kJ/kg}$
This is $< 50 \text{ kJ/kg}$
 $\Rightarrow \boxed{\text{Not possible}}$

③



Species	kmols	h_f°	$h - h_{298}$	S_i°	P_i	S_i
CO	1	-110,530	0	197.65	8	180.36
O ₂	1	0	0	205.04	1	205.04
CO ₂	1	-393,520	0	213.80	.667	217.17
O ₂	0.5	0	0	205.04	.333	214.18

$S_R = 385.40$

$S_o = 324.26$

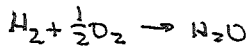
$h_R = -110,530$; $h_o = -393,520$

$W_{max} = h_R - h_o - T_o(S_R - S_o) = -110,530 - (-393,520) - (298)[385.4 - 324.26]$

$W_{max} = 264,770 \text{ kJ/kmole CO}$

or $\boxed{W_{max} = 264,770 \text{ kW}}$

④



$g - W = H_P - H_R$

Species	kmols	h_f°	$h - h_{298}$
H ₂	1	0	0
O ₂	0.5	0	0
H ₂ O	1	-241,820	$h_{H_2O} - 9904$

$-82,917 - 120,000 = -241,820 + h_{H_2O} - 9904 \Rightarrow h_{H_2O} = 48,807 \text{ kJ/kmole}$

$\Rightarrow \boxed{T_P = 1300 \text{ K}}$

ME 430/529 – Advanced Energy
Learning Objectives – Midterm Exam No. 2

Prior to the second exam (Tuesday, November 21), you should be able to:

1. Perform stoichiometry and energy balance calculations on real fuels (coal, biomass).
2. Perform calculations of real fuels in gasifiers.
3. Describe the major features of large-scale combustion/power plant technology.
4. Describe the sources and effects of the major pollutants, and perform calculations associated with the principal approaches to their control.
5. Find the energy released during radioactive decay reactions (both alpha and beta decay), and for fission reactions.
6. Determine radioisotope decay and calculate decay rates.
7. Describe features associated with the principal nuclear reactor systems and perform simple performance calculations.

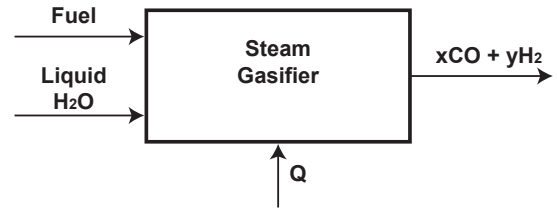
The exam will be open book and open notes (be sure to bring a thermo book). I will supply needed nuclear isotope half-life, decay pathway, and mass data. Your goal should be to understand the principles associated with Items 1-7 in a way that allows you to apply these to new problems. I suggest you study the homework solutions carefully if you have had any problems with the homework. Although the test is open book, if you need to do extensive reading of book or notes during the exam, or you attempt to follow a book example, you will probably have a time problem.

ME 430/529 – Advanced Energy
Example Midterm Exam

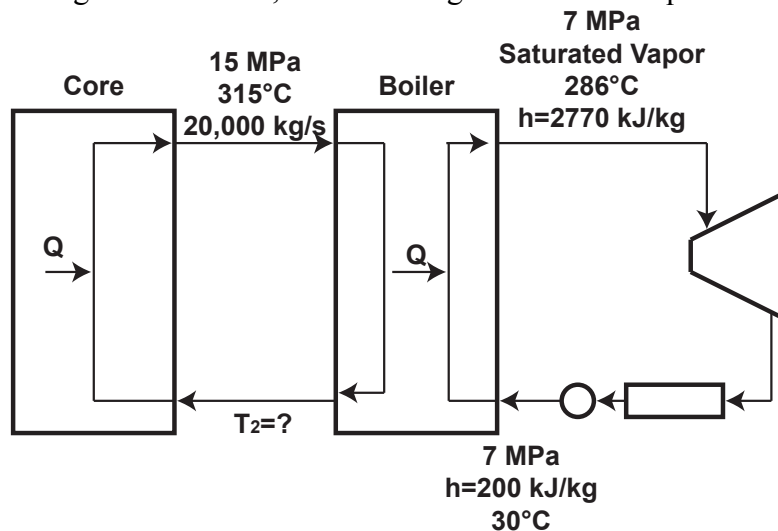
- 1.(35%) A biomass fuel has the following ultimate analysis:

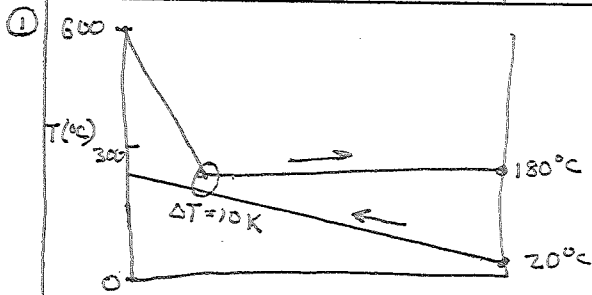
<u>Element</u>	<u>Mass Percent (as received)</u>
C	85.71%
H	14.29%

This fuel is converted in a steam gasifier with liquid water to produce CO and H₂. The fuel and the water enter the gasifier at 298 K. The products following the gasifier are cooled to 298 K. The LHV of the fuel is 15 MJ/kg. Find the amount of heat that must be supplied to the gasifier (MJ/kg fuel).



- 2.(30%) As mentioned in class, the only known example of natural fission was found in the Oklo uranium ore deposits in Gabon. The natural abundance of U-235 is 0.72%, the rest being U-238 (assume mole basis). This figure is quite constant world wide, except that the U-235 is depleted in this specific ore deposit. This is taken as evidence that infiltration of ground water into the uranium ore led to neutron moderation and a fission reaction in the distant past when U-235 was in higher concentration than today. Given that the half life of U-235 is $7.1\text{E}+8$ yr and that of U-238 is $4.51\text{E}+9$ yr, estimate the percent of total uranium that was U-235 at the time the fission was estimated to be active, $1.7\text{E}+9$ years ago.
- 3.(35%) The figure below shows the general schematic of a pressurized water reactor. For a limiting ΔT of 10 K within the boiler, find T_2 . You may use $\Delta h = C_p \Delta T$ for the pressurized water loop with $C_p = 4.2$ kJ/kg-K. At 7 MPa, $h = 1270$ kJ/kg for saturated liquid.





1st Law on condenser portion: Air T at pinch point = 170°C

$$\dot{m}_{\text{air}}(h_g - h_f) = \dot{m}_{\text{air}} C_p (T_{\text{pp}} - T_{\text{in}})$$

$$[1 \text{ kg/s}] [2777.1 - 762.5 \frac{\text{kJ}}{\text{kg}}] = \dot{m}_{\text{air}} [1 \frac{\text{kJ}}{\text{kg} \cdot \text{K}}] [170 - 20^\circ\text{C}]$$

$$\dot{m}_{\text{air}} = 13.43 \text{ kg/s}$$

1st Law on whole HX: $\dot{m}_{\text{st}}(h_{\text{in}} - h_{\text{f}}) = \dot{m}_{\text{air}} C_p (T_{\text{out}} - T_{\text{in}}) \Rightarrow [1] [3698.6 - 762.5] = [13.43] [T_{\text{out}} - 20] \Rightarrow T_{\text{out}} = 239^\circ\text{C}$

②

Element	Kg	Kmole
C	80	6.67
H	20	20

$$\Rightarrow 6.67\text{C} + 20\text{H} + \text{WO}_2 \rightarrow 6.67\text{CO} + 10\text{H}_2$$

$$\Rightarrow W = 3.33$$

$$\Rightarrow 1^{\text{st}} \text{ Law on gasifier } \dot{q} = H_P - H_R$$

Species	Kmole	h_f°
Fuel	100 kg	$h_{f,\text{fuel}}^\circ$
O ₂	3.33	0
CO	6.67	-110,530
H ₂	10	0

$$2,800,000 = [-110,530][6.67] - h_{f,\text{fuel}}^\circ$$

$$\Rightarrow h_{f,\text{fuel}}^\circ = -3,537,000 \text{ kJ/100 kg fuel}$$

Now burn the fuel: $6.67\text{C} + 20\text{H} + \text{WO}_2 \rightarrow 6.67\text{CO}_2 + 10\text{H}_2\text{O}$

O-atom: $2W = 2(6.67) + 10 \Rightarrow W = 11.67$

1st Law $\dot{q} = H_P - H_R$

Species	Kmole	h_f°
Fuel	100 kg	-3,537,000
O ₂	11.67	0
CO ₂	6.67	-393,520
H ₂ O(g)	10	-241,820

$$H_R = -3,537,000$$

$$H_P = -5,043,000$$

$$\dot{q} = -5,043,000 - (-3,537,000) = -1,506,000 \text{ kJ/100 kg fuel}$$

$$\text{LHV} = -\dot{q} \Rightarrow \text{LHV} = 15,060 \text{ kJ/kg fuel}$$

③

$$\frac{dN}{dt} = -\lambda N = -\frac{N}{\tau^*} \Rightarrow \tau^* = -\frac{N}{\left[\frac{dN}{dt}\right]}$$

$$\frac{dN}{dt} = -\frac{10 \text{ atoms}}{\text{s}}$$

$$N = \frac{1.0 \text{E-6 kg}}{200 \text{ kg}} \left| \frac{\text{kmole}}{\text{kg}} \right| \frac{6.023 \text{E+26 atoms}}{\text{kmole}} = 3.01 \text{E+18 atoms}$$

$$\tau^* = -\frac{3.01 \text{E+18 atoms}}{-10 \text{ atoms/s}} \left| \frac{\text{s}}{\text{yr}} \right| = 9.56 \text{E+9 yr}$$

$$\tau^* = -\frac{t_{1/2}}{\ln(0.5)} \Rightarrow t_{1/2} = -(\ln 0.5) \tau^* = -\ln(0.5) (9.56 \text{E+9 yr})$$

$$\Rightarrow t_{1/2} = 6.63 \text{E+9 yr}$$

**ME 430/529 – Advanced Energy
Learning Objectives – Final Exam**

Prior to the final exam (Tuesday, December 12, 2:30-4:30PM, MEB 248), you should be able to:

1. Perform performance calculations on combined cycle systems, including being able to identify whether a pinch-point violation is occurring within a HRSG.
2. Perform performance calculations on biomass-based gasification systems and integrated gasification combined cycle systems.
3. Find reversible energy release for fuel cells, and find theoretical cell voltages.
4. Evaluate reformer systems for making fuel cell fuels (e.g., H_2) in terms of their energy needs (exothermic and endothermic reactions) and their availability losses.

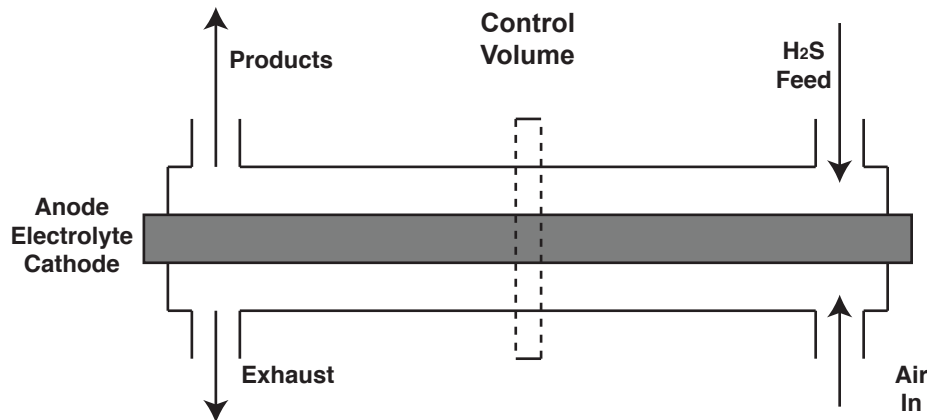
Items not listed above (e.g., fluidized beds, nuclear) will not explicitly appear on the exam. Some items (e.g., reaction stoichiometry balances) may be required as parts of other problems.

The exam will be open book and open notes (be sure to bring a thermo book). Your goal should be to understand the principles associated with Items 1-4 in a way that allows you to apply these principles to new problems. I suggest you study the homework solutions carefully if you have had any problems with the homework. Although the test is open book, if you need to do extensive reading of books or notes during the exam, or you attempt to follow a book example, you will probably have a time problem.

ME 430/529 – Advanced Energy
Example Final Exam

- 1.(35%) A fuel cell uses H_2S (hydrogen sulfide) as a fuel and air as the oxidizer. The products are SO_2 and H_2O . At the point indicated in the figure as the control volume (CV), the mole fraction of the O_2 on the oxidizer side is 0.1. On the anode side, half the H_2S has reacted away at the CV point. The electrolyte transmits O^{2-} (oxygen ions with a double negative charge), just like a solid oxide fuel cell. The temperature is 298 K and the pressure is 1 atm everywhere. Assume H_2O is a vapor. Find the theoretical cell voltage at the CV point.

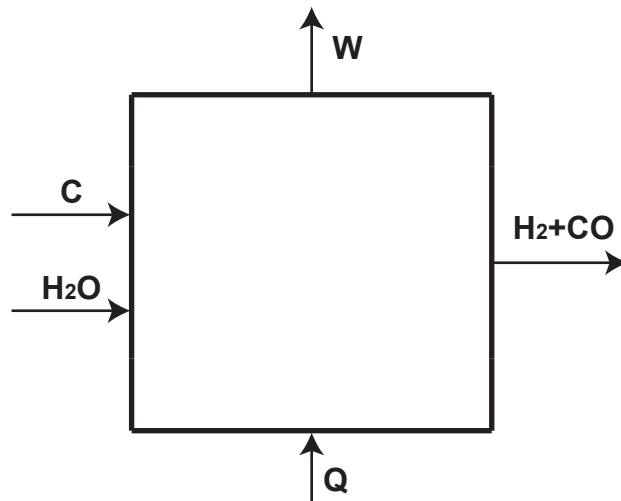
	h_f^0 , kJ/kmole	s^0 , kJ/kmole-K
H_2S	-20,600	205.81
SO_2	-296,810	248.22
H_2O	-241,820	188.83
O_2	0.0	205.04
N_2	0.0	191.61

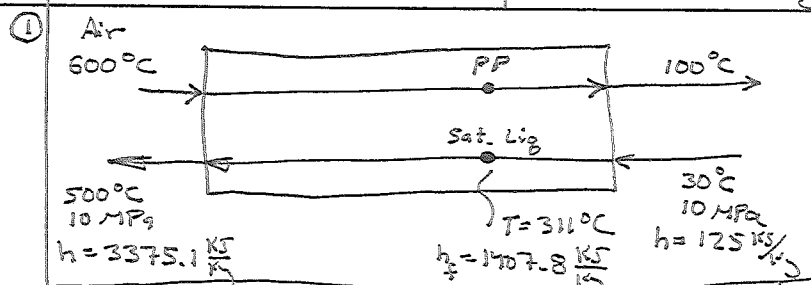


- 2.(30%) You have a 100 kg/s stream of air available at 1 atm and 773 K. This is to be used as a heat source for a Rankine cycle via an HRSG. The condenser in the Rankine cycle is at 10 kPa and produces a saturated liquid. This gives the following conditions at the pump outlet: $h=201.9$ kJ/kg, $s=0.6492$ kJ/kg-K, $T=46^\circ\text{C}$. The Rankine boiler pressure is 10 MPa. Choose parameters (i.e., temperatures) for your HRSG which are (1) economically realistic, and (2) minimize the irreversibility of the HRSG so far as is economically reasonable (document these). Then find the irreversibility of the HRSG (kW). ($T_0=298$ K, $P_0=1.0$ atm.)

- 3.(35%) A gasification system accepts graphite (C) and liquid water at 298 K and 1 atm, and produces a mixed stream of CO and H₂, also at 298 K and 1 atm. The process can be thought of as a “black box” that contains many parts, but you are asked to find the minimum amount of work flow into the process that is necessary for the process to proceed (kJ/kmole graphite). Note that in the figure, I have drawn the Q and W with our usual sign conventions, but that they may have negative values in reality.

	h_f^0 , kJ/kmole	s^0 , kJ/kmole-K
C	0.0	5.74
H ₂ O(f)	-285,830	69.92
CO	-110,530	197.65
H ₂	0.0	130.68





• Assume basis of 1 kg for air
 • 1st Law on whole system:
 $m_a C_p (T_{in} - T_{out}) = m_{st} (h_{out} - h_{in})$
 $(1)(1)(600 - 100) = m_{st} (3375.1 - 125)$
 $\Rightarrow m_{st} = 0.1538 \text{ kg}$

• 1st Law on FWH: $m_a C_p (T_{PP} - T_{out}) = m_{st} (h_f - h_{in})$
 $(1)(1)(T_{PP} - 100) = (0.1538)(1407.8 - 125) \Rightarrow T_{PP} = 297^\circ\text{C}$
 $S_o: T_{PP} < 311^\circ\text{C} \Rightarrow \text{PP Violation}$
 $\Rightarrow \text{Not possible}$

②

14 kg biomass $\Rightarrow$ 12 kg C + 2 kg H $\Rightarrow$ 1 kmole C + 2 kmols H
 Get h_f° for fuel:

$$C + 2H + wO_2 \rightarrow CO_2 + H_2O \Rightarrow w = 3/2$$

$$g = -LHV = \frac{-18,000 \text{ kJ} / 14 \text{ kg}}{\text{kg}} = -252,000 \text{ kJ}$$

$$g = H_P - H_R \Rightarrow -252,000 = -393,520 - 241,820 - H_R$$

$$\Rightarrow H_R = h_f^\circ = -383,340 \text{ kJ} / 14 \text{ kg}$$

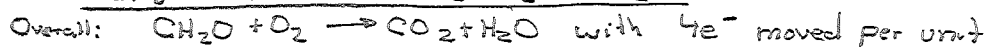
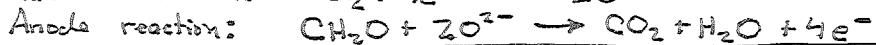
Reformer: $g = H_P - H_R$ $C + 2H + yO_2 \rightarrow CO + H_2 \Rightarrow y = 0.5$

$$0 = g = -110,530 - [-383,340 + h_{O_2}]$$

$$\Rightarrow T_3 = 15,800 \text{ K}$$

$$[0.5 \text{ kmols}] [1.1 \frac{\text{kJ}}{\text{kg-mol}}] [32 \text{ kg/kmole}] (T_3 - 298)$$

③



stoichiometry -

• Products appear on cathode side.

$\Rightarrow O_2$ partial pressure stays as 1 atm.

• Assume 1 kmole of CH_2O to start. At 50% point have 0.5 kmols CH_2O

- Carbon balance gives 0.5 kmols CO_2

- Hydrogen balance gives 0.5 kmols H_2O

$$\Rightarrow P_{CH_2O} = P_{CO_2} = P_{H_2O} = 0.333 \text{ atm.}$$

Species	Kmols	h_f°	S_i°	P_i	S_i
CH_2O	1	-115,900	218.95	0.33	228.17
O_2	1	0	205.04	1	205.04
CO_2	1	-393,520	213.80	0.33	223.02
H_2O	1	-241,820	188.83	0.33	198.05

$$S_R = 433.21$$

$$S_P = 421.07$$

$$H_R = -115,900$$

$$H_P = -635,340$$

(note I am including the P_i correction in the original Wrev equation)

$$W_{rev} = H_R - H_P - T_0 (S_R - S_P) = -115,900 - (-635,340) - (298) [433.21 - 421.07]$$

$$= 515,822 \text{ kJ/kmole}$$

$$\frac{515,822 \text{ kJ} / 10^3 \text{ J} / \text{kmole}}{\text{kmole}} \frac{\text{kJ}}{\text{kmole}} \frac{\text{kmole}}{4 \text{ kmols } e^-} \frac{\text{kmole } e^-}{9.64 \times 10^4 \text{ coul}} \Rightarrow E^\circ = 1.338 \text{ V}$$